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**A Boundary Element Method Formulation Based on the Caputo Derivative
for the Solution of the Anomalous Diffusion Problem**

by

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Abstract

This work presents a Boundary Element Method formulation for the solution of the anomalous diffusion problem. By keeping the fractional time derivative as it appears in the governing differential equation of the problem, and by employing a Weighted Residual Method approach with the steady state fundamental solution for anisotropic media playing the role of the weighting function, one obtains the boundary integral equation of the proposed formulation. The presence of a domain integral with the fractional time derivative as part of its integrand, and the evaluation of this fractional time derivative as a Caputo derivative, constitute the main feature of the formulation. The analyses of some examples, in which the numerical results are always compared with the corresponding analytical solutions, show the robustness of the formulation, as accurate results are obtained even for small values of the order of the time derivative.

1. Introduction

Great deal of attention has been given to the solution of problems governed by partial differential equations containing non-integer derivatives, as attested by the work by Sun et al. [1], in which various applications are listed. Such kind of problems belong to the domain of the so-called *fractional calculus*, although, according to Miller and Ross [2], the use of the word fractional is a misnomer, as generalized operators can include rational or irrational, positive or negative, real or complex orders. Despite this caveat, this nomination will be kept here, as it is found in textbooks, e.g. Ortigueira [3], due to the tradition attached to its use.

This work is concerned with the solution of the anomalous diffusion equation for two-dimensional problems, assuming anisotropic media, by a Boundary Element Method (BEM) formulation. The anomalous, or fractional, diffusion equation presents a time-derivative of order α , with $0 < \alpha < 1$. From this point of view, the classical diffusion equation, for which $\alpha = 1$, can be looked upon as a particular case of a most general problem represented by the fractional diffusion equation. The time-derivative of order α , called from now on as fractional time-derivative, can be represented either by the Caputo or by the Riemann-Liouville operators; in fact, these are integro-differential operators, differing one from the other according to the sequence of the execution of the operations of derivation and integration. When the initial conditions are zero, the definitions coincide, see Ortigueira [3], Gorenflo and Mainardi [4].

In a previous but related work, the authors presented another BEM formulation based on the use of the Riemann-Liouville derivative: in that approach, by means of an inverse operation involving both the Riemann-Liouville and the Caputo derivatives, see Ortigueira [3], an ordinary time-derivative of order one replaces the fractional time-derivative that, by its turn, is transferred to the Laplacian; the interested reader is referred to Carrer et al. [5] for additional details concerning this matter. Now, in this work, a new BEM formulation is developed in which the fractional time-derivative is kept unaltered, that is to say, the formulation is developed by using the Caputo derivative directly. This is the main feature of the formulation and, most probably, the feature that rendered its robustness: while the previous formulation, named FD-BEM, failed to produce useful results for $\alpha < 0.5$, the new formulation is prone to produce accurate results even for very small values of α : indeed, in all examples results for $\alpha = 0.05$, that are in a good agreement with the analytical solutions, are presented. As before, the proposed formulation employs the fundamental solution of the steady-state problem and, for this reason, it is of the type D-BEM. Due to the use of the Caputo derivative, it will be called, from now on, CD-BEM, with C meaning Caputo and D meaning domain; note that this designation tacitly states that the formulation is concerned with the anomalous diffusion equation. As the fractional differential operators are non-local – this meaning that the determination of a future state of a given system depends not only on the current but on all

the previous states – a summation term, representing the history contribution, appears in the CD-BEM equation. This summation term turns the CD-BEM formulation more time consuming than the standard D-BEM formulation, see the Examples. In Riemann-Liouville based formulations, e.g. Carrer et al. [5], Yuste and Acedo [6], a strong dependency of the time-step, Δt , with respect to the order α of the fractional derivative is observable. This dependency is such that in the concluding remarks of reference [6] one can read: “the number of steps needed to reach even moderate time would become prohibitively large’. The CD-BEM formulation, on the other hand, does not present such a strong dependency between Δt and α . Consequently, regardless of the value of α , the same time-step could be used in all the analyses for each example. This is a favourable aspect of the CD-BEM formulation that renders it attractive.

The integrand of the domain integral in the CD-BEM equation is constituted by the product of the fractional time derivative with the fundamental solution of the steady-state classical diffusion problem. To compute this integral, it is assumed that the Caputo fractional time derivative varies linearly in the triangular cells of the domain discretization, and that the variable of interest, say u , varies linearly in each time-step. The boundary discretization, by its turn, employs linear elements. Under these assumptions, boundary and domain integrations are carried out following standard BEM procedures. After the assemblage of the matrices, the time-marching process can start. Note that the standard D-BEM formulation arises when $\alpha = 1.0$

Four examples are included in which the BEM results are always compared with the analytical solution. Accurate results were obtained for α ranging from 1.0 to 0.05.

Although the fractional calculus is as old as the standard calculus, presently it is considered an emerging field in mathematics and in many branches of science and engineering where non-locality plays an important role. As the number of applications has increased, a great deal of attention has been given to the development of numerical methods for the solution of fractional differential equations. Diverse BEM approaches can be found, for instance: Katsikadelis [7] employed the concept of an analog equation together with the BEM to solve two-dimensional problems, and Dehghan and Safarpour [8], presented a dual reciprocity BEM formulation. In what concerns the Finite Difference Method (FDM), a great number of articles can be found and, among them, the works by Meerschaert and Tadjeran [9], Langlands and Henry [10], Yuste and Acedo [6], Tadjeran and Meerschaert [11], Murio [12], Murillo and Yuste [13], Li et al. [14], Çelic and Duman [15], Li and Li [16], Sousa and Li [17] can be cited. In what concerns the Finite Element Method (FEM), one can cite the works by Roop [18], Agrawal [19], Deng [20], Huang et al. [21], Zheng et al. [22], Ainsworth and Glusa [23], Esen et.al [24].

In addition to the classic methods, other techniques were presented: for example, meshless formulations can be seen in Kumar et al. [25], Shekari et al. [26] and Zafarghandi et al. [27], and the

reproducing kernel algorithm formulation can be found in Arqub and Shawagfeh [28], and Arqub [29], whereas and residual power series approach can be found in Arqub [31]. Naturally, this is only a little survey concerning a research area that increases continuously. In this context, the authors intend to demonstrate that their new BEM approach, or rather, the CD-BEM formulation, can be used as a powerful tool for the solution of anomalous diffusion problems.

2. The Anomalous Diffusion Problem

The anomalous diffusion problem, in the Caputo sense, for anisotropic media, is governed by the equation:

$$\frac{\partial_c^\alpha u}{\partial t^\alpha} = D_x \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} D_y \quad (1)$$

where $0 < \alpha < 1$, and D_x and D_y are the constant diffusion coefficients in x and y directions, respectively.

For a domain Ω , with the boundary Γ represented as: $\Gamma = \Gamma_u \cup \Gamma_q$, the boundary conditions are then schematically defined as follows:

$$\text{Dirichlet boundary condition: } u(X, t) = \hat{u}(X, t), \text{ over } \Gamma_u \quad (2)$$

and

$$\text{Neumann boundary condition: } q(X, t) = D_x \frac{\partial u}{\partial x} n_x + D_y \frac{\partial u}{\partial y} n_y = \hat{q}(X, t), \text{ over } \Gamma_q \quad (3)$$

In Equation (3), n_x and n_y are the components of the unit outward normal vector to the boundary.

The initial condition is defined as:

$$u(X, 0) = u_0(X) \quad (4)$$

In equations (2), (3) and (4), X represents the point of coordinates (x, y) , that is, $X = (x, y)$.

The fractional derivative of α -order with respect to time that appears on the left-hand-side of Equation (1) is known as the Caputo derivative and is defined as:

$$\frac{\partial_c^\alpha u}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{1}{(t-\tau)^\alpha} \frac{\partial u(\tau)}{\partial \tau} d\tau \quad (5)$$

Unlike the authors' previous formulation, see Carrer et al. [5], the development of the new BEM formulation, to be presented below, starts directly from Equation (1), without any manipulation in its original form.

3. The Boundary Element Method

The Weighted Residuals Method, e.g., Brebbia et al. [31], Zienkiewicz and Morgan [32], is used as the starting point for the development of the basic Boundary Element Method (BEM) integral equation. Here, the fundamental solution of the steady-state classical diffusion problem, say w , plays the role of the weighting function for the domain residuals. The weighting functions for the residuals at the boundaries Γ_u and Γ_q , denoted here, respectively, as \bar{w} and $\overline{\bar{w}}$ are determined in such a way that unnecessary approximations to the boundary conditions are avoided.

The weighted residual equation is written as:

$$\int_{\Omega} \left[\frac{\partial_{\mathbf{c}}^{\alpha} u}{\partial t^{\alpha}} - \left(D_x \frac{\partial^2 u}{\partial x^2} + D_y \frac{\partial^2 u}{\partial y^2} \right) \right] w d\Omega + \int_{\Gamma_u} (u - \hat{u}) \bar{w} d\Gamma + \int_{\Gamma_q} (q - \hat{q}) \overline{\bar{w}} d\Gamma = 0 \quad (6)$$

After applying the divergence theorem, the functions \bar{w} and $\overline{\bar{w}}$ are chosen to avoid approximations to the boundary conditions. In this way, one has:

$$\bar{w} = - \left(D_x \frac{\partial^2 w}{\partial x^2} + D_y \frac{\partial^2 w}{\partial y^2} \right) = Q \quad (7)$$

and

$$\overline{\bar{w}} = w \quad (8)$$

Remembering that:

$$D_x \frac{\partial^2 w}{\partial x^2} + D_y \frac{\partial^2 w}{\partial y^2} = -\delta(X - \xi), \quad (9)$$

the substitution of Equations (7) – (9) into Equation (6) produces a BEM equation valid, however, only for $\xi \in \Omega$. In order to solve the problem numerically, the limiting form of such a BEM equation, in which $\xi \rightarrow \Gamma$, should be obtained. This is done following standard procedures, such as that presented by Brebbia et al. [31], and the resulting equation, called the basic BEM equation reads:

$$c(\xi)u(\xi, t) = \int_{\Gamma} q(X, t)w(\xi, X)d\Gamma(X) - \int_{\Gamma} u(X, t)Q(\xi, X)d\Gamma(X) - \int_{\Omega} \frac{\partial_c^\alpha u(X, t)}{\partial t^\alpha} w(\xi, X)d\Omega(X) \quad (10)$$

In equation (10), $\xi = (\xi_x, \xi_y)$ and $X = (x, y)$ are called, respectively, *source* point and is the *field* point.

The term $c(\xi)$ appears as a consequence of the limiting process mentioned above. For $\xi \in \Omega$, it is assumed that $c(\xi) = 1$. For $\xi \in \Gamma$, $c(\xi)$ is computed according to, see Carrer et al. [33]:

$$c(\xi) = \frac{1}{2\pi} \left[\tan^{-1} \left(\sqrt{\frac{D_x}{D_y}} \tan \theta_2 \right) - \tan^{-1} \left(\sqrt{\frac{D_x}{D_y}} \tan \theta_1 \right) \right] \quad (11)$$

The angles θ_1 and θ_2 in Equation (11) are depicted in Figure 1.

The fundamental solution is given by, see Berger and Karageorghis [34]:

$$w = w(\xi, X) = -\frac{1}{2\pi\sqrt{D_x D_y}} \ln \sqrt{(x - \xi_x)^2 + \frac{D_x}{D_y} (y - \xi_y)^2} \quad (12)$$

For isotropic media, $D_x = D_y = D$ and expressions (11) and (12) become the well-known expressions below, see:

$$w(\xi, X) = -\frac{1}{2\pi D} \ln \sqrt{(x - \xi_x)^2 + (y - \xi_y)^2} = -\frac{1}{2\pi D} \ln r \quad (13)$$

and

$$c(\xi) = \frac{\theta_2 - \theta_1}{2\pi} \quad (14)$$

BEM formulations concerned with the solution of time-dependent problems can be developed using non-time-dependent fundamental solutions, thus generating the so-called D-BEM formulations. The letter D, in this case, stands for domain, indicating the presence of a domain integral in the BEM integral equations. The kernel of such domain integrals is constituted by the product of the fundamental solution with the time derivative of the variable of interest, u , or any other function that can be treated as a domain body force. For the present case, the product of the

fundamental solution by the fractional time derivative of u constitutes the kernel of the domain integral. Based on this discussion, the formulation developed here can be named CD-BEM, with the letter C standing for the Caputo derivative, which means that it is concerned with the solution of a fractional problem.

For computational purposes, the variable t in Equation (10) is replaced by a discrete value, say $t_{n+1} = (n+1)\Delta t$, where Δt is the selected time interval, and $0 \leq t \leq t_{n+1}$. Also, aiming at computing the integral in Equation (5) analytically, it is assumed that u varies linearly between two consecutive time steps. By adopting a simplified notation, in which: $u_k = u(X, t_k) = u_k(X)$, one has:

$$u = \frac{(t_{k+1} - \tau)}{\Delta t} u_k + \frac{(\tau - t_k)}{\Delta t} u_{k+1} \quad (15)$$

and consequently:

$$\frac{\partial u}{\partial \tau} = \frac{u_{k+1} - u_k}{\Delta t} \quad (16)$$

Finally, the resulting expression for the Caputo derivative can be written as:

$$\left. \frac{\partial_C^\alpha u}{\partial t^\alpha} \right|_{t=t_{n+1}} = \frac{1}{\Gamma(1-\alpha)} \left[\int_0^{t_1} \frac{1}{(t_1 - \tau)^\alpha} \frac{(u_1 - u_0)}{\Delta t} d\tau + \int_{t_1}^{t_2} \frac{1}{(t_2 - \tau)^\alpha} \frac{(u_2 - u_1)}{\Delta t} d\tau + \dots + \int_{t_k}^{t_{k+1}} \frac{1}{(t_{k+1} - \tau)^\alpha} \frac{(u_{k+1} - u_k)}{\Delta t} d\tau + \dots + \int_{t_n}^{t_{n+1}} \frac{1}{(t_{n+1} - \tau)^\alpha} \frac{(u_{n+1} - u_k)}{\Delta t} d\tau \right] \quad (17)$$

After performing all the integrations in Equation (17), the resulting expression can be written as:

$$\left. \frac{\partial_C^\alpha u}{\partial t^\alpha} \right|_{t=t_{n+1}} = \frac{1}{\Gamma(2-\alpha)\Delta t^\alpha} \left[u_{n+1} - u_n + \sum_{j=0}^{n-1} \left(\frac{1}{(n+1-j)^{\alpha-1}} - \frac{1}{(n-j)^{\alpha-1}} \right) (u_{j+1} - u_j) \right] \quad (18)$$

More concisely, Equation (18) can be rewritten as:

$$\left. \frac{\partial_C^\alpha u}{\partial t^\alpha} \right|_{t=t_{n+1}} = \frac{1}{\Gamma(2-\alpha)\Delta t^\alpha} \left[u_{n+1} - u_n + \sum_{j=0}^{n-1} B_{(n+1),(j+1)} (u_{j+1} - u_j) \right] \quad (19)$$

where:

$$B_{(n+1),(j+1)} = \frac{1}{(n+1-j)^{\alpha-1}} - \frac{1}{(n-j)^{\alpha-1}} \quad (20)$$

Note that Equation (18) is valid for $n \geq 1$. When $n = 0$, it is written simply as:

$$\left. \frac{\partial_c^\alpha u}{\partial t^\alpha} \right|_{t=t_1} = \frac{1}{\Gamma(2-\alpha)\Delta t^\alpha} [u_1 - u_0] \quad (21)$$

Equation (18) now can be substituted into Equation (10), and the resulting expression is:

$$\begin{aligned} c(\xi)u_{n+1}(\xi) &= \int_{\Gamma} q_{n+1}(X)w(\xi, X)d\Gamma(X) - \int_{\Gamma} u_{n+1}(X)Q(\xi, X)d\Gamma(X) - \\ &\frac{1}{\Gamma(2-\alpha)\Delta t^\alpha} \int_{\Omega} \left[u_{n+1}(X) - u_n(X) + \sum_{j=0}^{n-1} B_{(n+1),(j+1)} (u_{j+1}(X) - u_j(X)) \right] w(\xi, X) d\Omega(X) \end{aligned}$$

For the computation of the boundary integrals in Equation (22), linear elements were employed in the boundary discretization, assuming a linear variation to u and q in each element. The computation of the domain integral requires the discretization of the entire domain. Linear triangular cells were employed in the domain discretization, with the assumption of linear variation for u in the cells. The matrix form of Equation (21) is written as:

$$\begin{aligned} \begin{bmatrix} \mathbf{H}^{bb} & \mathbf{0} \\ \mathbf{H}^{db} & \mathbf{I} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_{n+1}^b \\ \mathbf{u}_{n+1}^d \end{Bmatrix} &= \begin{bmatrix} \mathbf{G}^{bb} \\ \mathbf{G}^{db} \end{bmatrix} \left\{ \mathbf{q}_{n+1}^b \right\} - \begin{bmatrix} \mathbf{M}^{bb} & \mathbf{M}^{bd} \\ \mathbf{M}^{db} & \mathbf{M}^{dd} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_{n+1}^b - \mathbf{u}_n^b \\ \mathbf{u}_{n+1}^d - \mathbf{u}_n^d \end{Bmatrix} - \\ \begin{bmatrix} \mathbf{M}^{bb} & \mathbf{M}^{bd} \\ \mathbf{M}^{db} & \mathbf{M}^{dd} \end{bmatrix} \sum_{j=0}^{n-1} B_{(n+1),(j+1)} \begin{Bmatrix} \mathbf{u}_{j+1}^b - \mathbf{u}_j^b \\ \mathbf{u}_{j+1}^d - \mathbf{u}_j^d \end{Bmatrix} \end{aligned} \quad (23)$$

After rearranging the common terms, Equation (23) can be written as:

$$\begin{aligned} \begin{bmatrix} (\mathbf{H}^{bb} + \mathbf{M}^{bb}) & \mathbf{M}^{bd} \\ (\mathbf{H}^{db} + \mathbf{M}^{db}) & (\mathbf{I} + \mathbf{M}^{dd}) \end{bmatrix} \begin{Bmatrix} \mathbf{u}_{n+1}^b \\ \mathbf{u}_{n+1}^d \end{Bmatrix} &= \begin{bmatrix} \mathbf{G}^{bb} \\ \mathbf{G}^{db} \end{bmatrix} \left\{ \mathbf{q}_{n+1}^b \right\} + \begin{bmatrix} \mathbf{M}^{bb} & \mathbf{M}^{bd} \\ \mathbf{M}^{db} & \mathbf{M}^{dd} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_n^b \\ \mathbf{u}_n^d \end{Bmatrix} - \\ \begin{bmatrix} \mathbf{M}^{bb} & \mathbf{M}^{bd} \\ \mathbf{M}^{db} & \mathbf{M}^{dd} \end{bmatrix} \sum_{j=0}^{n-1} B_{(n+1),(j+1)} \begin{Bmatrix} \mathbf{u}_{j+1}^b - \mathbf{u}_j^b \\ \mathbf{u}_{j+1}^d - \mathbf{u}_j^d \end{Bmatrix} \end{aligned} \quad (24)$$

The unknown values of u and q , at time t_{n+1} , are determined after applying the boundary conditions to Equation (24). Note that: *i*) the non-local behaviour of the Caputo fractional operator is characterized by the summation symbol in Equations (22) and in Equations (23) and (24): the computation of the current values of u and q depends not only on their current values, but also on all the previous values of u , that is, depends on the history; *ii*) the last term on the right hand side of Equation (24) is null when $\alpha = 1.0$, as this case corresponds the BEM formulation for the classical diffusion problem. In Equations (23) and (24), superscripts b and d correspond to the boundary and domain variables, while the double superscripts are related to the positions of the source and field points: the first superscript indicates the position of the former, the second, the position of the latter. The identity matrix \mathbf{I} is related to points that belong to the domain; as already mentioned, for such points $c(\xi) = 1$.

Note that Equation (23) is much simpler than the corresponding matrix equation presented by Carrer et al. [5], in which the history contribution takes into account all the previous values of u and q .

4. Examples

In this section, the CD-BEM formulation is validated. Four examples are included and discussed. For each example, the BEM results are presented as functions of time or of the spatial coordinates and are always compared with the analytical solutions. This comparison showed that reliable results, even for small values of α such as $\alpha = 0.2$ and $\alpha = 0.05$, are furnished by the CD-BEM formulation. Besides the analyses with these two small values of α , other analyses were also carried out, with $\alpha = 1.0$, that corresponds to the classical diffusion problem, and with $\alpha = 0.8$ and with $\alpha = 0.5$.

The BEM results were obtained from a computer program developed by the authors, written in the language Fortran 90. The structure of such a computer program is quite simple and its steps are listed below:

- a) Input data concerning the geometry: number of nodes and their coordinates; number of linear boundary elements, n_{Γ} , and of linear triangular cells, n_{Ω} ; connectivity of the boundary elements and of the cells;
- b) Input data concerning the boundary conditions;
- c) Input data concerning the time-step Δt , the number of time-steps, and the order α of the time derivative;
- d) Input data concerning the media: D_x and D_y ;
- e) Assemblage of the matrices that appear in Equation (24);
- f) Beginning of the time marching process: if $\alpha = 1$, the summation operation indicated in Equations (24) is avoided;
- g) Print the results for the select node as a function of time;
- h) Print the results for the geometry for the selected times.

4.1. Rectangular Domain with sinusoidal initial condition

This example presents a bar with length $L = \pi$, with an initial condition given by:

$$u_0(x) = \sin x \quad (25)$$

The boundary conditions, assuming $0 \leq x \leq \pi$, then are: $u(0,t) = 0$ and $u(\pi,t) = 0$.

The analytical solution for an isotropic medium with $D_x = D_y = D = 1.0$ reads, see Murillo and Yuste [13]:

$$u_0(x) = E_\alpha(-t^\alpha) \sin x \quad (26)$$

In equation (26), $E_\alpha(\dots)$ is the Mittag-Leffler function, defined according to:

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1 + \alpha k)} \quad (27)$$

where $z \in \mathbb{C}$, $\Gamma(\dots)$ is the gamma function, and α is the fractional order of the derivative. If $\alpha = 1.0$, Equation (27) reduces to:

$$E_1(z) = e^z \quad (28)$$

and equation (26) becomes the well-known classical diffusion equation analytical solution. From this point of view, this analytical solution can be looked upon as a particular case of the solution given by equation (26).

The two-dimensional analysis of this one-dimensional problem was carried out in a rectangular domain defined on the region $0 \leq x \leq \pi$ and $0 \leq y \leq \pi/2$, with the Dirichlet boundary conditions:

$$u(0, y, t) = u(\pi, y, t) = 0 \quad (29)$$

and with the Neumann boundary conditions below, chosen to turn possible the simulation of the one-dimensional problem:

$$q(x, 0, t) = q(x, \pi/2, t) = 0 \quad (30)$$

The initial condition is:

$$u_0(x, y) = \sin x \quad (31)$$

The BEM analyses employed the mesh depicted in Figure 2. That mesh contains $n_T = 48$ linear elements of the same length and $n_\Omega = 256$ linear triangular cells of the same area. Figure 3 depicts the results for u as a function of time at the point $(x, y) = (\pi/2, \pi/4)$. Good agreement between the BEM results and the analytical solution is observed for the chosen values of α , that is, the proposed formulation was prone to provide accurate results **for** the classical diffusion problem and **for the** anomalous diffusion problem with very low orders of the time derivative. Besides, and this a very important aspect to be mentioned here, while the previous formulation presented by Carrer et al. [5] failed for $\alpha < 0.5$, this new formulation provides accurate results even for small values of α , such as $\alpha = 0.2$ and $\alpha = 0.05$.

In what concerns the choice of the time-step, this is a crucial matter for this kind of problem; bearing in mind the critical time-step proposed by Yuste and Acedo [6] for a Finite Difference Method approach, and given by:

$$\Delta t^\alpha \leq \frac{D\Delta x^2}{2^{2-\alpha}} \quad (32)$$

one can see how advantageous the CD-BEM formulation is, as it does not present such a strong dependence of Δt with respect to the order α of the time derivative. Indeed, the same time-step, $\Delta t = 0.005$, was employed in all analyses.

In Figures 4 and 5 one finds the results for u as a function of x for the selected instants of time, **that is, for $t = 0.25$** and $t = 2.0$. As expected, good agreement is observed between the BEM results and the analytical solution for all values of α .

The computer time is a matter that deserves attention due to the non-local behaviour of the fractional operators or, bearing in mind Equations (22 – 24), due to the summation term that takes into account the history contribution in the computation of the values of u and q for each time. The CPU time required for the solution **of the** classical diffusion problem, say $t_{CPU}^{\alpha=1}$, can be regarded as the reference CPU time; consequently, the ratio between the CPU times for the fractional analyses, t_{CPU}^α , and $t_{CPU}^{\alpha=1}$ provides a measure of how the fractional analyses increase the **required** computer time. Here, one has:

$$\frac{t_{CPU}^{\alpha}}{t_{CPU}^{\alpha=1}} = 97 \quad (33)$$

Note that the CPU time is related only on the marching process and does not include the time for assembling the matrices, as this time is the same regardless the value of α . For this first example, $t_{CPU}^{\alpha=1.0} = 3.015s$.

4.2. Rectangular Domain with Dirichlet boundary conditions

This second example also deals with a one-dimensional problem: now, the problem interpreted as that of a heat transfer from the region at $x = 0$ to the region at $x = L$ is analysed in a rectangular domain, defined on the region $0 \leq x \leq L$ and $0 \leq y \leq L/2$. The mesh is that already employed in the first example, scaled to accommodate the different domain size, as now one has $L = 2$.

The Dirichlet boundary conditions are:

$$u(0, L/2, t) = 10 \quad (34)$$

$$u(L, y, t) = 0 \quad (35)$$

The Neumann boundary conditions:

$$q(x, 0, t) = q(x, L/2, t) = 0 \quad (36)$$

enable the simulation of the one-dimensional problem.

The initial condition is null, that is,

$$u_0(x, y) = 0 \quad (37)$$

The analyses were carried out with $D_x = D_y = D = 1.0$. Following the same sequence of the previous example, results for u at $(x, y) = (L/2, L/4)$, as a function of time, are presented in Figure 6. Results for u , for the selected instants of time $t = 0.25$ and $t = 1.0$, are presented in Figures 7 and 8, respectively. All the analyses were carried out with the same time-step, $\Delta t = 0.005$. Again, good agreement is observed between BEM results and the analytical solution, given by:

$$u(x, t) = U_0 \left(1 - \frac{x}{L} \right) - \frac{2U_0}{\pi} \sum_{k=1}^{\infty} \frac{1}{k} E_{\alpha} \left(- \left(\frac{k\pi}{L} \right)^2 D t^{\alpha} \right) \sin \left(\frac{k\pi x}{L} \right) \quad (38)$$

The solution given by expression (38) cannot be evaluated using expression directly (26), because the argument of the Mittag-Leffler function grows faster than its convergence radius. To overcome this difficulty, the Mittag-Leffler function was computed through the algorithm found at

<https://github.com/khinsen/mittag-leffler>, which is a Python language version of a MATLAB[®] routine presented by Garrappa [35].

Regarding the reference CPU time, now one has $t_{CPU}^{\alpha=1.0} = 1.12s$. and:

$$\frac{t_{CPU}^{\alpha}}{t_{CPU}^{\alpha=1.0}} = 57 \tag{39}$$

4.3. Circular Domain with Dirichlet Boundary Condition

This example presents a circular domain, conveniently described in the polar coordinate system (r, θ) , with $0 \leq r \leq R$ and $0 \leq \theta \leq 2\pi$.

With zero initial condition, $u_0(R, \theta) = 0$, and the Dirichlet boundary condition:

$$u(R, \theta, t) = \hat{u} \quad (40)$$

the problem becomes axisymmetric for an isotropic medium. The governing equation of the problem, Equation (1), is rewritten as:

$$\frac{\partial^\alpha u}{\partial t^\alpha} = D \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} \right) \quad (41)$$

From equation (41) $u = u(r, t)$.

The analytical solution reads:

$$u(r, t) = \hat{u} - \frac{2\hat{u}}{R} \sum_{n=1}^{\infty} \frac{J_0(\lambda_n r)}{\lambda_n J_1(\lambda_n R)} E_\alpha(-D\lambda_n^2 t) \quad (42)$$

where $J_0(\dots)$ and $J_1(\dots)$ are the Bessel functions of the first kind and orders zero and one, respectively, and the parameters λ_n are the positive roots of the equation

$$J_0(\lambda_n R) = 0 \quad (43)$$

The analyses were carried out with the parameters $D = 1.0$, $R = 10$ and $\hat{u} = 10$. Three meshes, with increasing level of discretization, were employed to investigate the convergence of the BEM results to the analytical solution through the computation of the relative L^2 error norm, E_2 . **The convergence is guaranteed as the error norm diminishes with the increasing level of refinement.** The first mesh presents the poorest discretization, with $n_T = 16$ and $n_\Omega = 144$, see Figure 9. For this mesh, $\Delta t = 0.8$. The second mesh, see Figure 10, has $n_T = 32$ and $n_\Omega = 544$ and the time-step is $\Delta t = 0.4$. The third and more refined mesh, depicted in Figure 11, has $n_T = 64$ and $n_\Omega = 2368$. The time step is $\Delta t = 0.2$. From now on, these meshes will be called, respectively, as mesh 1, 2 and 3.

The results for E_2 , computed according to:

$$E_2 = \frac{\|u_{analytical} - u_{BEM}\|_{L^2(\Omega)}}{\|u_{analytical}\|_{L^2(\Omega)}} \quad (44)$$

are presented in Figures 12 and 13 for $t = 8.0$ and $t = 20.0$. It can be observed, in Figures 12 and 13, a significant reduction in the error with the mesh refinement. Indeed, more refined meshes are required to obtain accurate results for smaller values of α . A quite similar convergence pattern was also observed for other values of time and, for this reason, the results presented here were restricted to $t = 8.0$ and $t = 20.0$. Also, it is important to mention that the error decreases as the time increases, that is, as the problem approaches the steady-state condition; see, for instance, Figure 14, with the results for $\alpha = 0.5$ for $t = 4.0, 8.0, 12.0, 20.0$.

Results for u as a function of r , for selected instants of time, are depicted in Figures 15 – 19 for $\alpha = 1.0, 0.8, 0.5, 0.2, 0.05$, respectively, with $t = 1.0, 4.0, 20.0, 60.0$, and results for u at $r = 5$ as a function of t are depicted in Figure 20. The last six figures provide a good description of how the results are influenced by the parameter α . It can be seen, in Figures 15 – 19, that decreasing the values of α results in decreasing the values of u , for $r < R$, with the curves for different times becoming closer to each other and presenting increasing gradients towards the boundary: this description is better illustrated for the results corresponding to $\alpha = 0.05$. Regarding Figure 20, it is observed that more and more time is required to reach the steady state as α decreases. As an overall conclusion, the BEM results are in good agreement with the analytical solution.

For this example, the results regarding the CPU time are summarized in Table 1. Note that the ratios in the third column refer to the same mesh. This observation is also valid for Table 2, in the next example.

Table 1. Circular domain: CPU times.

mesh	$t_{CPU}^{\alpha=1.0}$ (sec.)	$t_{CPU}^{\alpha} / t_{CPU}^{\alpha=1.0}$
1	0.094	4.0
2	0.626	25.0
3	32,782	40.0

4.4. Square domain with initial sinusoidal condition

A square domain defined in the region $0 \leq x, y \leq L$, with the boundary conditions:

$$u(0, y, t) = u(L, y, t) = u(x, 0, t) = u(x, L, t) = 0 \quad (45)$$

and the initial condition:

$$u_0(x, y) = \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \quad (46)$$

is analysed next. The side of the square is $L = 10$.

For anisotropic media, the analytical solution is given by:

$$u(x, y, t) = E_\alpha(-v^2 t) \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \quad (47)$$

with:

$$v = \frac{\pi}{L} \sqrt{D_x + D_y} \quad (48)$$

The results for an isotropic medium, with $D_x = D_y = 1.0$, and for an anisotropic medium, with $D_x = 1.0$ and $D_y = 0.1$, are presented next. Three meshes were employed to verify the convergence of the BEM results to the analytical solution at times $t = 10$ and $t = 15$. The first mesh has $n_\Gamma = 40$ and $n_\Omega = 200$, the second $n_\Gamma = 80$ and $n_\Omega = 800$. The third mesh, depicted in Figure 21, has $n_\Gamma = 160$ and $n_\Omega = 3200$. These meshes will be referred to as mesh 1, mesh 2, and mesh 3, for which $\Delta t = 0.2, 0.1, 0.05$, respectively.

The errors for the selected values of α can be seen in Figures 22 and 23 for the isotropic medium, and in Figures 24 and 25 for the anisotropic medium. From these figures it is readily seen that the BEM results converge to the analytical solution, with the errors decreasing as more refined meshes are employed. For the isotropic medium, Figures 22 and 23 show different convergence paths regarding the pure diffusion and the anomalous diffusion problems: quite unexpectedly, the errors associated with $\alpha = 1.0$ range from the smallest, with mesh 1, to the biggest ones, with

meshes 2 and 3. For $\alpha < 1$, one can observe that, with the mesh 1, the errors decrease insofar as the values of α decrease and become practically the same with meshes 2 and 3, with the smallest errors being related to $\alpha = 0.8$. Regarding the anisotropic medium, Figures 24 and 25 show similar convergence paths for all the values of α . Note that the errors for $\alpha = 1.0$ are the biggest ones with mesh 1, then becomes the smallest ones with mesh 2, and with mesh 3 the errors for all the values of α are practically the same.

Accurate results for $u(L/2, L/2, t)$ are depicted in Figures 26 and 27, for isotropic and anisotropic media, respectively. The independence of Δt regarding α is observed again. In Figures 28, for isotropic medium, and 29, for anisotropic medium, u is presented as a function of the position for $t = 10$.

Table 2 presents a comparison between the CPU times.

Table 2. Square domain: CPU times.

mesh	$t_{CPU}^{\alpha=1.0}$ (sec.)	$t_{CPU}^{\alpha} / t_{CPU}^{\alpha=1.0}$
1	0.172	15.0
2	2.8	50.0
3	118.	108.0

Conclusions

The main contribution of this work, its novelty, is the development of a BEM formulation for the solution of the anomalous diffusion problem: this formulation, called for general purposes CD-BEM, proved to be capable of producing accurate and reliable results even for small values of the order of the time derivative, represented by the Greek letter α . Indeed, a value so small as $\alpha = 0.05$ was employed and the numerical results presented a good agreement with the analytical solution. Note that the solution of problems presenting such a small value of α are hardly found in the literature concerning numerical methods. The Caputo derivative was kept as it appeared in the governing differential equation of the problem and this approach brought many advantages, such as the storage of only the previous values of the variable of interest, u , in the computation of the history contribution for the present state of the problem. An important advantage, from the computation point of view, is that the choice of the time-step was not so strongly dependent on the order of the time derivative, rendering the analyses less time consuming than those based on the use of the Riemann-Liouville approach previously presented by the authors. But the main advantage brought by the proposed formulation is the possibility of analyzing problems with small values of α , enabling the authors to state that the CD-BEM formulation is capable of covering all the range $0 < \alpha < 1.0$ that characterizes the anomalous diffusion problem. The development of a D type formulation seemed to be the natural choice, in the absence, as long as the authors know, of a proper fundamental solution. Naturally, development the results presented here encourage further developments and these could be the implementation of more accurate approximations for the Caputo derivative in the domain integral, the use of time-steps with variable lengths and, mainly, the development of a similar formulation for the solution of the wave-diffusion problem, for which $1 < \alpha < 2$. The CD-BEM formulation also demonstrates that the Boundary Element Method can be used as a powerful tool for the solution of fractional calculus problems.

The development of a BEM formulation concerned with the solution of the anomalous diffusion equation for **two-dimensional problems is the main contribution, is the novelty, of this work**. The use of the Weighted Residuals Method as the initial step towards the development of this formulation seems to be advantageous, according to the authors' previous experience in dealing with this kind of problems, with the resulting BEM integral equation easily obtained. In the absence of a proper fundamental solution, the steady-state fundamental solution played the role of the weighting function, resulting in a D-BEM type formulation. Called CD-BEM for general purposes, this formulation is based on the direct use of the Caputo derivative. Thanks to this approach, the computation of the variables u and q at the present time requires the storage of only the values of u

at the previous times to take into account the history contribution, diversely from the Riemann-Liouville based formulation, for which the history contribution employed the previous values of both variables u and q . Note that due to the non-local behaviour of the fractional operators, the computational of the history contribution is required, which turns the analyses of this kind of problems quite expensive from the computational point of view. Here, another advantage of the CD-BEM formulation appears, that is, the choice of the time-step is not so strongly dependent on the order of the time derivative as it was in the Riemann-Liouville approach previously presented by the authors. In fact, all the analyses in each example were carried out with the same time-step, regardless the value of α . But the main advantage brought by the proposed formulation is the possibility of analyzing problems with small values of α . Indeed, a value so small as $\alpha = 0.05$ was employed and the numerical results presented a good agreement with the analytical solution. Note that the solution of problems presenting such a small value of α are hardly found in the numerical methods literature, encouraging the authors to state that the CD-BEM formulation is capable of covering all the range $0 < \alpha \leq 1.0$, the inclusion of the equality sign in the range of the variable α being justified since the classical diffusion problem is considered as a particular case of the anomalous diffusion. Finally, the results presented here encourage further developments and these could be the implementation of more accurate approximations for the Caputo derivative in the domain integral, the use of time-steps with variable lengths and, mainly, the development of a similar formulation for the solution of the wave-diffusion problem, for which $1 < \alpha < 2$. The CD-BEM formulation also demonstrates that the Boundary Element Method can be used as a powerful tool for the solution of fractional calculus problems.

The development of a BEM formulation concerned with the solution of the anomalous diffusion equation for **two-dimensional problems is the main contribution, the novelty, of this work**. The use of the Weighted Residuals Method as the initial step towards the development of this formulation seems to be advantageous, according to the authors' previous experience in dealing with this kind of problems, with the resulting BEM integral equation easily obtained. In the absence of a proper fundamental solution, that is to say, of a fundamental solution for the anomalous diffusion equation, the fundamental solution of steady-state classical diffusion problem plays the role of the weighting function, resulting in a D-BEM type formulation. Called CD-BEM for general purposes, this formulation is based on the direct use of the Caputo derivative. Thanks to this approach, in order to take into account the history contribution, which is required for the computation of the variables u and q at the present time, only the values of u at the previous times are employed and, consequently, require storage, diversely from the authors' Riemann-Liouville based formulation, for which the history contribution computation requires the storage of the previous values of both variables u and

q. Note that the history contribution computation is required due to the non-local behaviour of the fractional operators, which turns the analyses of this kind of problems quite expensive from the computational point of view. Here, another advantage of the CD-BEM formulation appears, that is, the choice of the time-step is not so strongly dependent on the order of the time derivative as it was in the Riemann-Liouville approach previously presented by the authors. In fact, all the analyses in each example were carried out with the same time-step, regardless the value of α . But the main advantage brought by the proposed formulation is the possibility of analyzing problems with small values of α . Indeed, a value so small as $\alpha = 0.05$ was employed and the numerical results presented a good agreement with the analytical solution. Note that problems presenting such a small value of α are hardly found in the numerical methods literature, encouraging the authors to state that the CD-BEM formulation is capable of covering all the range $0 < \alpha \leq 1.0$, the inclusion of the equality sign being justified since the classical diffusion problem can be treated as a particular case of the anomalous diffusion problem. Finally, the results presented here encourage further developments and, among these, the implementation of more accurate approximations for the Caputo derivative in the domain integral, the use of time-steps with variable lengths and, mainly, the development of a similar formulation for the solution of the wave-diffusion problem, for which $1 < \alpha < 2$, should be cited. The CD-BEM formulation also demonstrates that the Boundary Element Method can be used as a powerful tool for the solution of fractional calculus problems.

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Caption to the Figures

Figure 1. Identification of the angles for the computation of $c(\xi)$.

Figure 2. Mesh with $n_\Gamma = 48$ and $n_\Omega = 256$ employed in the first and in the second examples.

Figure 3. Domain under initial condition: results for $u(\pi/2, \pi/4, t)$.

Figure 4. Domain under initial condition: results for $u(x, \pi/4, 0.25)$.

Figure 5. Domain under initial condition: results for $u(x, \pi/4, 2.0)$.

Figure 6. Domain with Dirichlet boundary conditions: results at $u(L, L/2, t)$.

Figure 7. Domain with Dirichlet boundary conditions: results at $u(x, L/2, 0.25)$.

Figure 8. Domain with Dirichlet boundary conditions: results at $u(x, L/2, 1.0)$.

Figure 9. Circular domain: mesh 1 with $n_\Gamma = 16$ and $n_\Omega = 144$.

Figure 10. Circular domain: mesh 2 with $n_\Gamma = 32$ and $n_\Omega = 544$.

Figure 11. Circular domain: mesh 3 with $n_\Gamma = 64$ and $n_\Omega = 2368$.

Figure 12. Circular domain: convergence study for $t = 8.0$.

Figure 13: Circular domain: convergence study for $t = 20.0$.

Figure 14: Circular domain: convergence study for $\alpha = 0.5$.

Figure 15: Circular domain: results for $u(r, t_s)$, with $t_s = 1.0, 4.0, 20.0, 60.0$ and $\alpha = 1.0$.

Figure 16: Circular domain: results for $u(r, t_s)$, with $t_s = 1.0, 4.0, 20.0, 60.0$ and $\alpha = 0.8$.

Figure 17: Circular domain: results for $u(r, t_s)$, with $t_s = 1.0, 4.0, 20.0, 60.0$ and $\alpha = 0.5$.

Figure 18: Circular domain: results for $u(r, t_s)$, with $t_s = 1.0, 4.0, 20.0, 60.0$ and $\alpha = 0.2$.

Figure 19: Circular domain: results for $u(r, t_s)$, with $t_s = 1.0, 4.0, 20.0, 60.0$ and $\alpha = 0.05$.

Figure 20: Circular domain: results for $u(5, t)$.

Figure 21. Square Domain: mesh 3 with $n_\Gamma = 160$ and $n_\Omega = 3200$.

Figure 22. Square Domain: isotropic medium, convergence study for $t = 10.0$.

Figure 23. Square Domain: isotropic medium, convergence study for $t = 15.0$.

Figure 24. Square Domain: anisotropic medium, convergence study for $t = 10.0$.

Figure 25. Square Domain: anisotropic medium, convergence study for $t = 15.0$.

Figure 26. Square domain: isotropic medium, results for $u(L/2, L/2, t)$.

Figure 27. Square domain: anisotropic medium, results for $u(L/2, L/2, t)$.

Figure 28. Square domain: isotropic medium, results for $u(x, L/2, 10)$.

Figure 29. Square domain: isotropic medium, results for $u(x, L/2, 10)$.

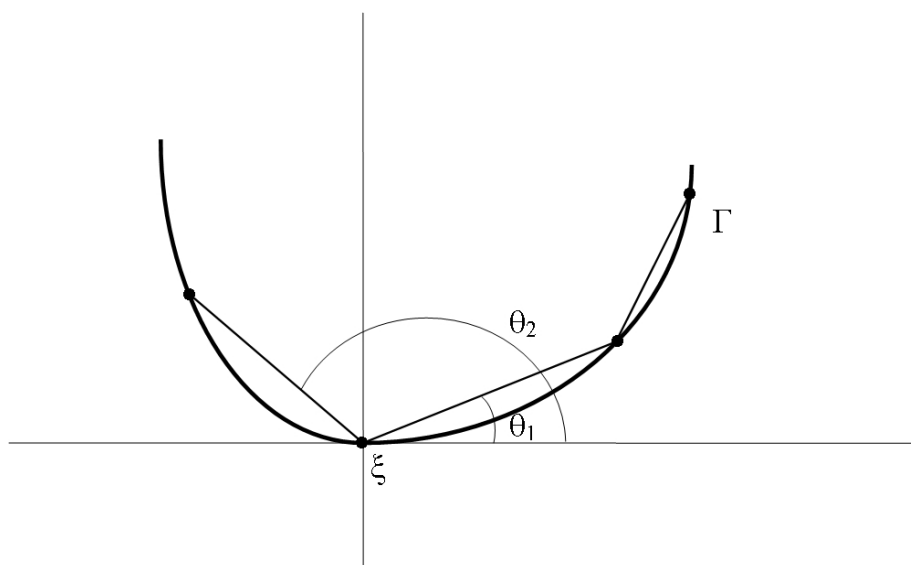


Figure 1

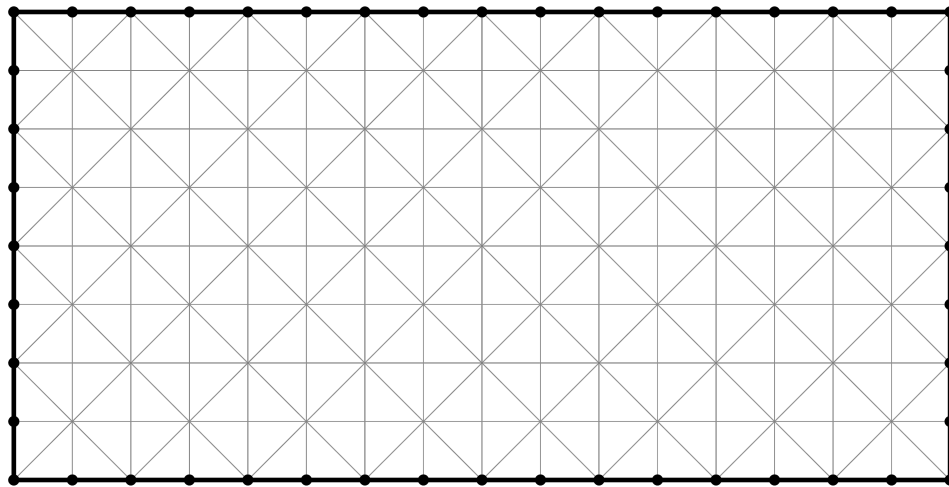


Figure 2

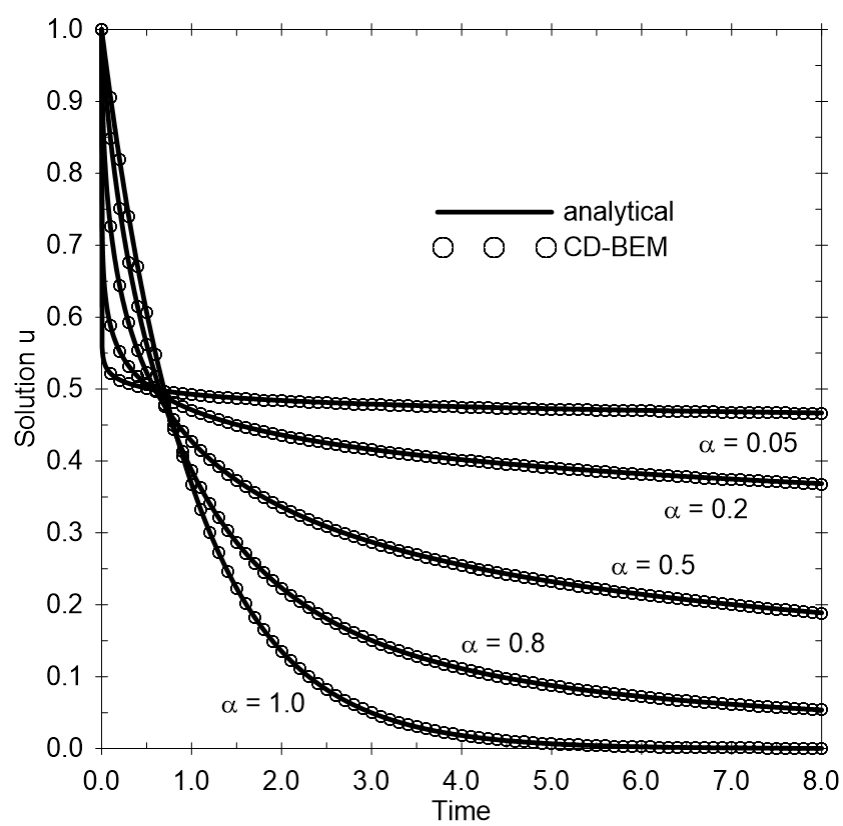


Figure 3

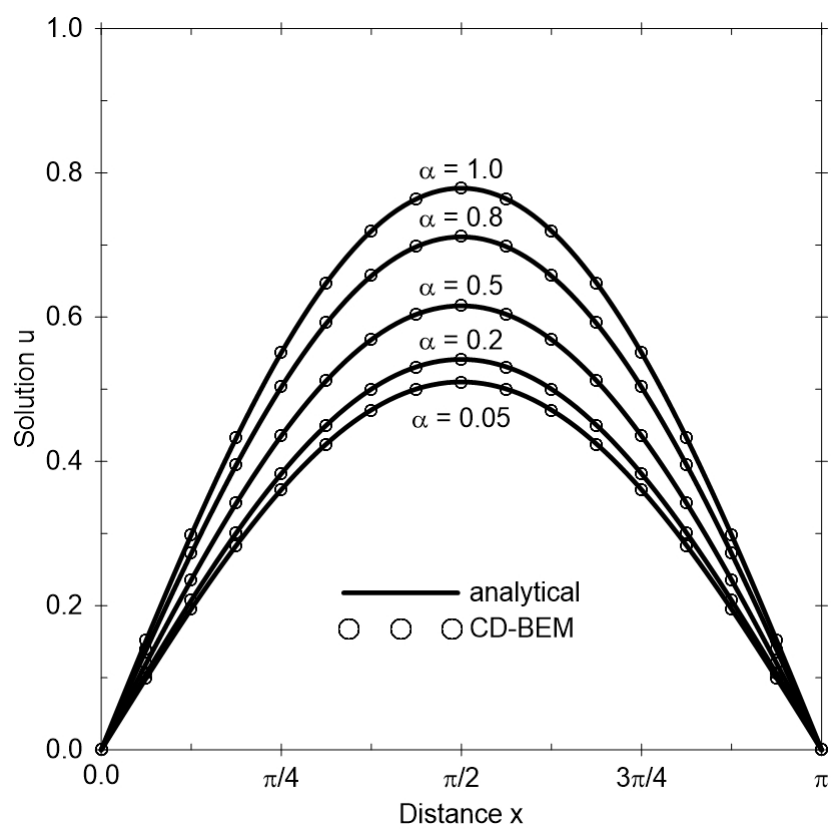


Figure 4

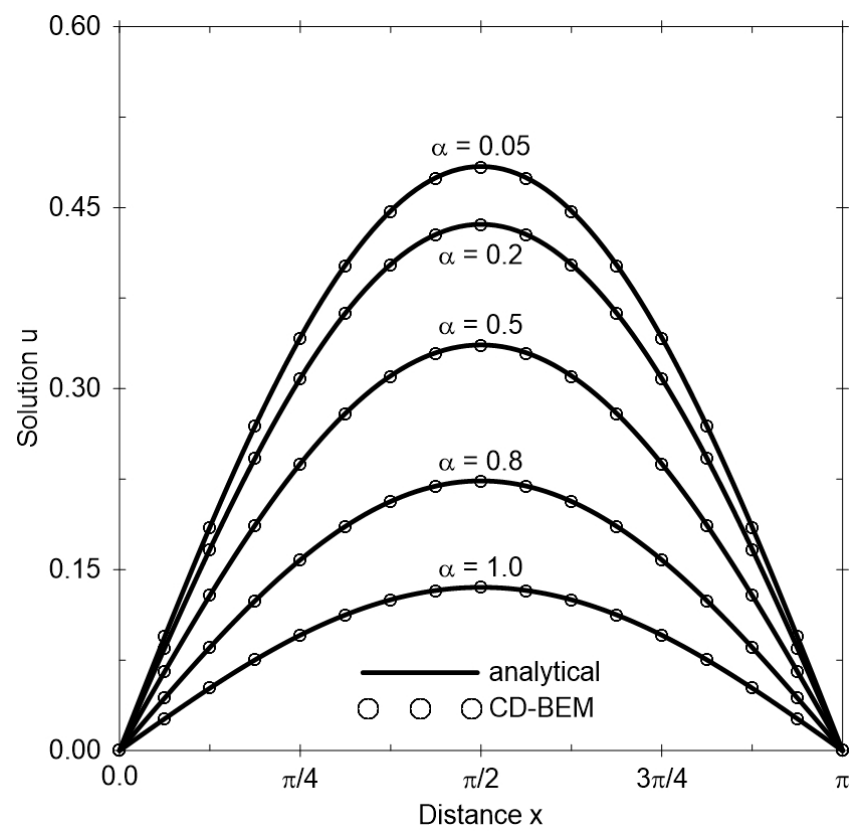


Figure 5

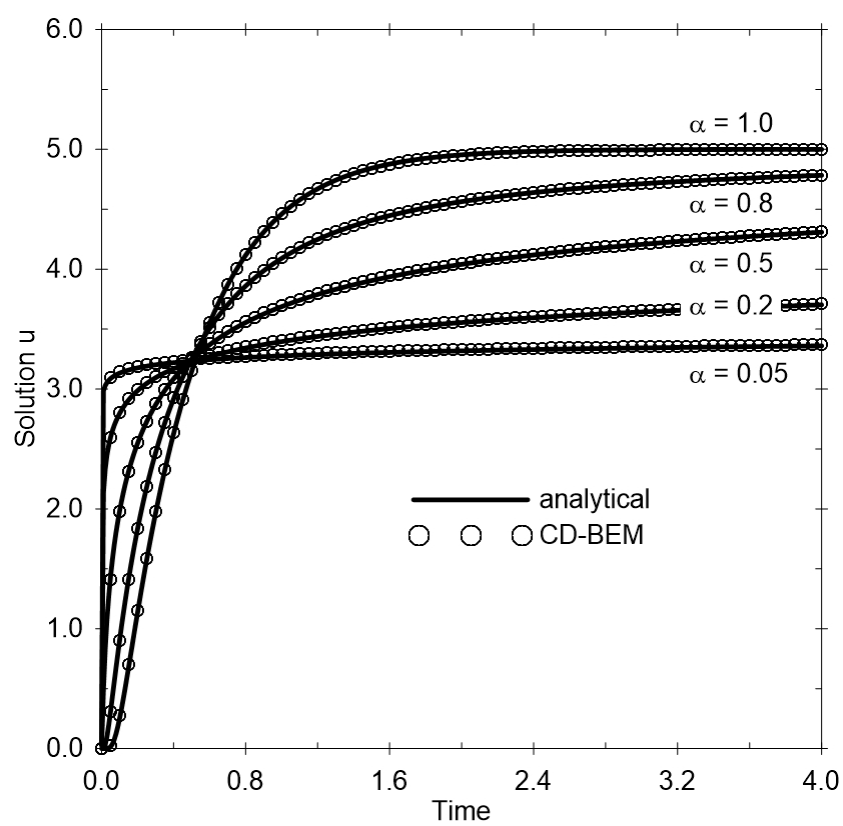


Figure 6

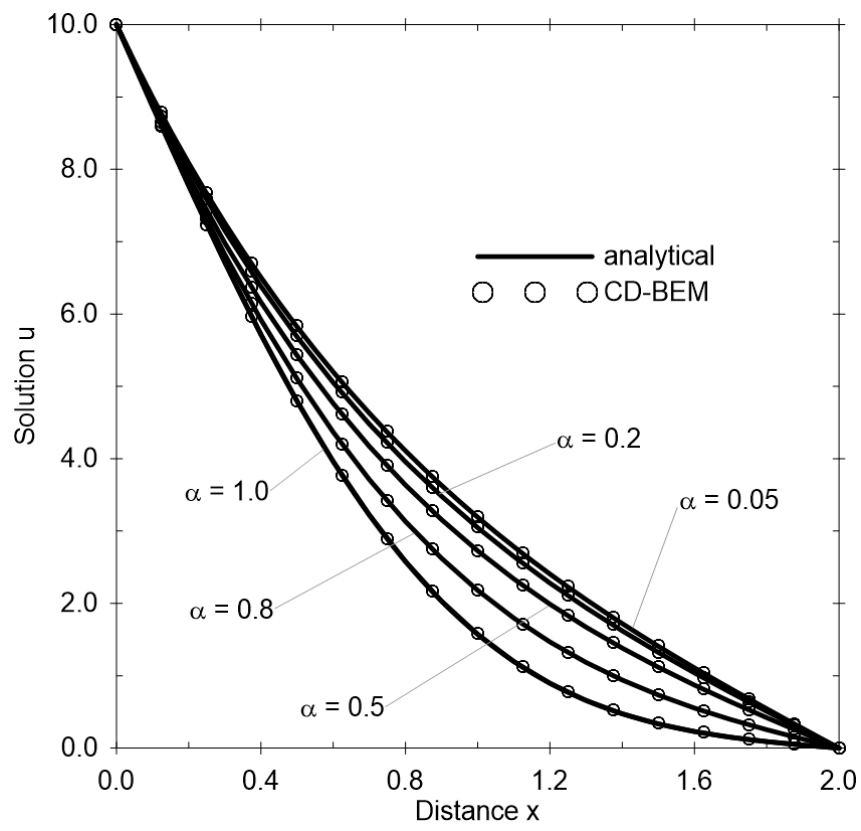


Figure 7

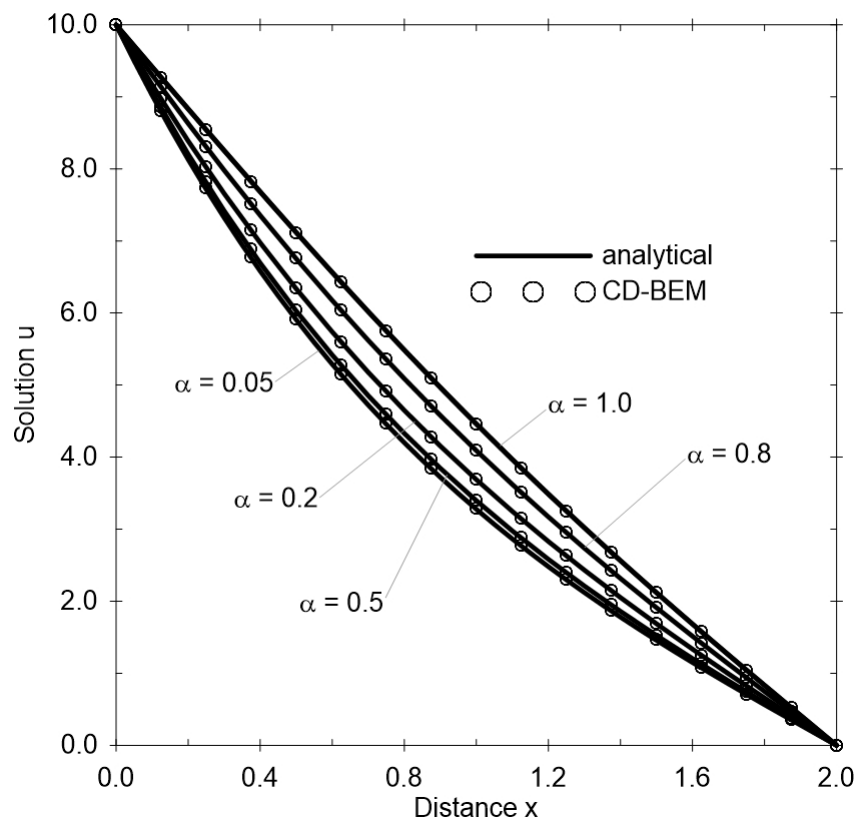


Figure 8

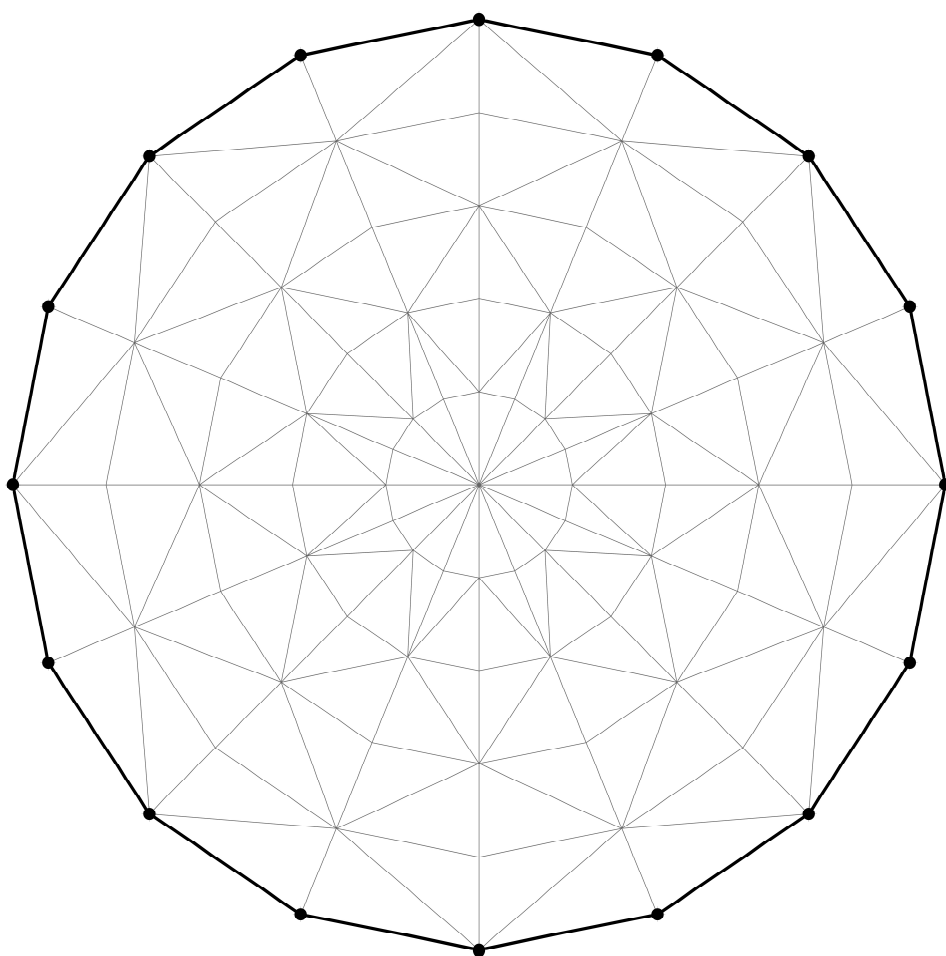


Figure 9

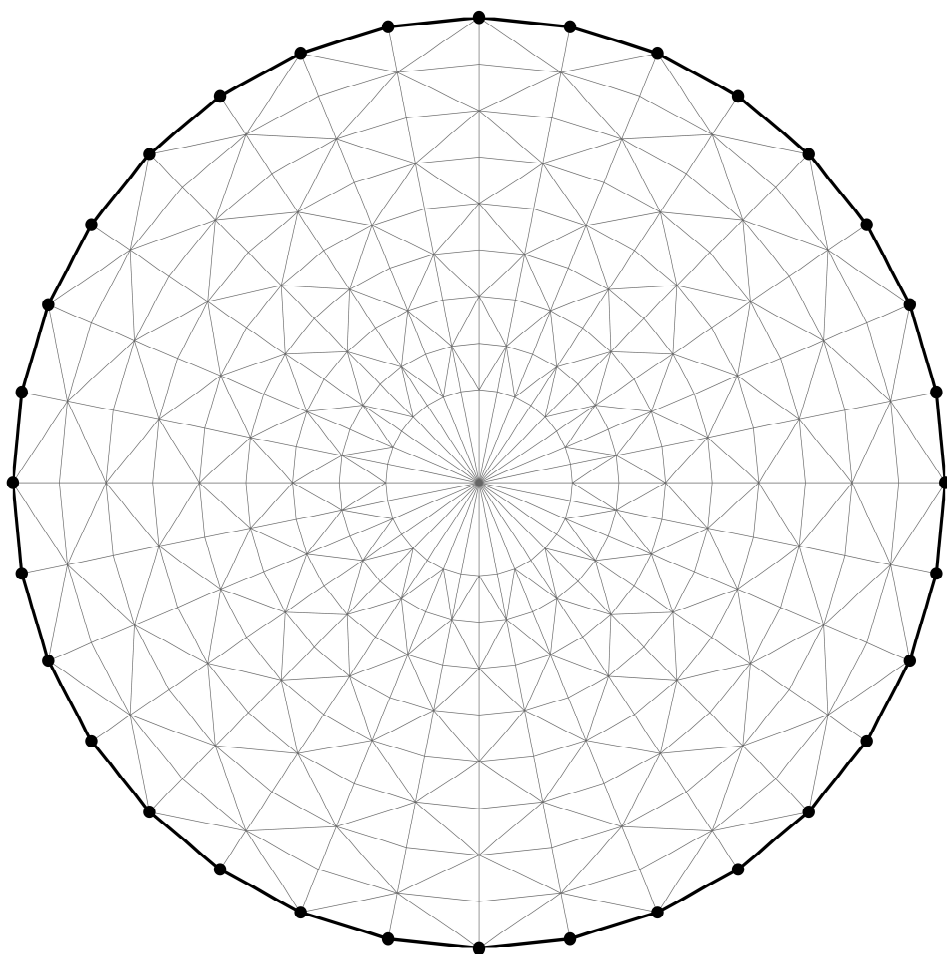


Figure 10

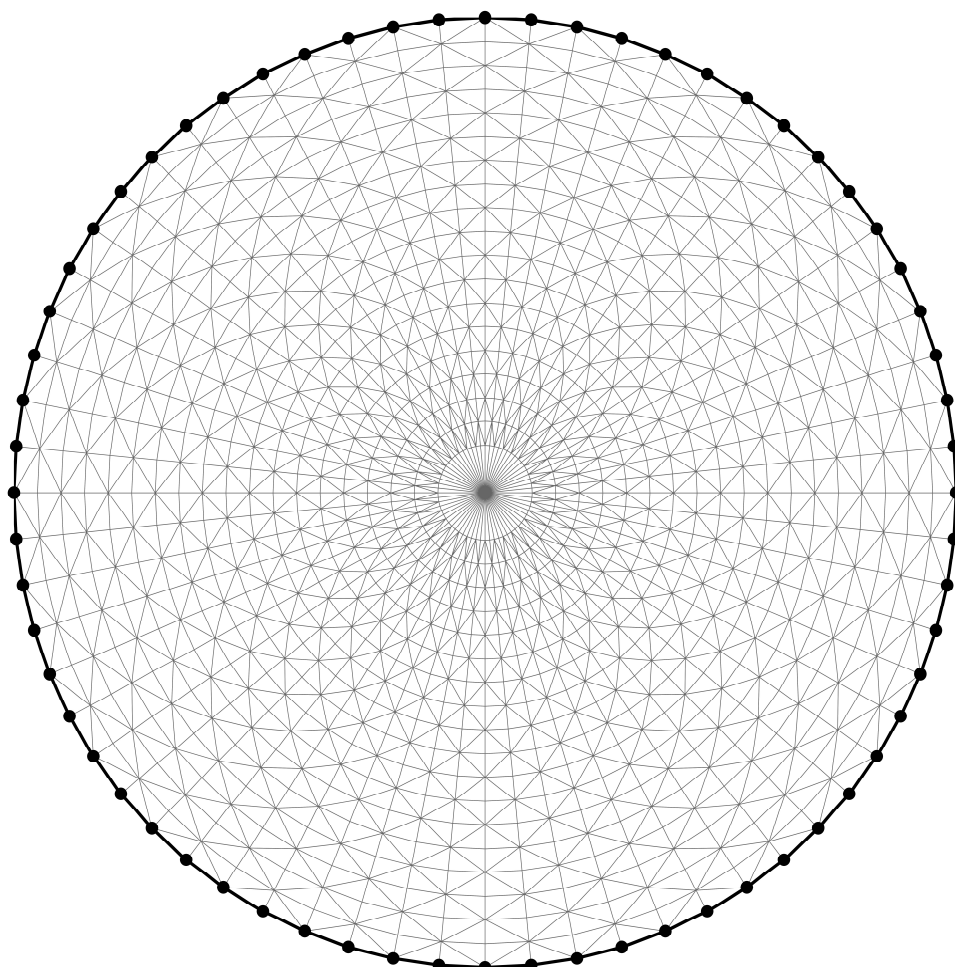


Figure 11

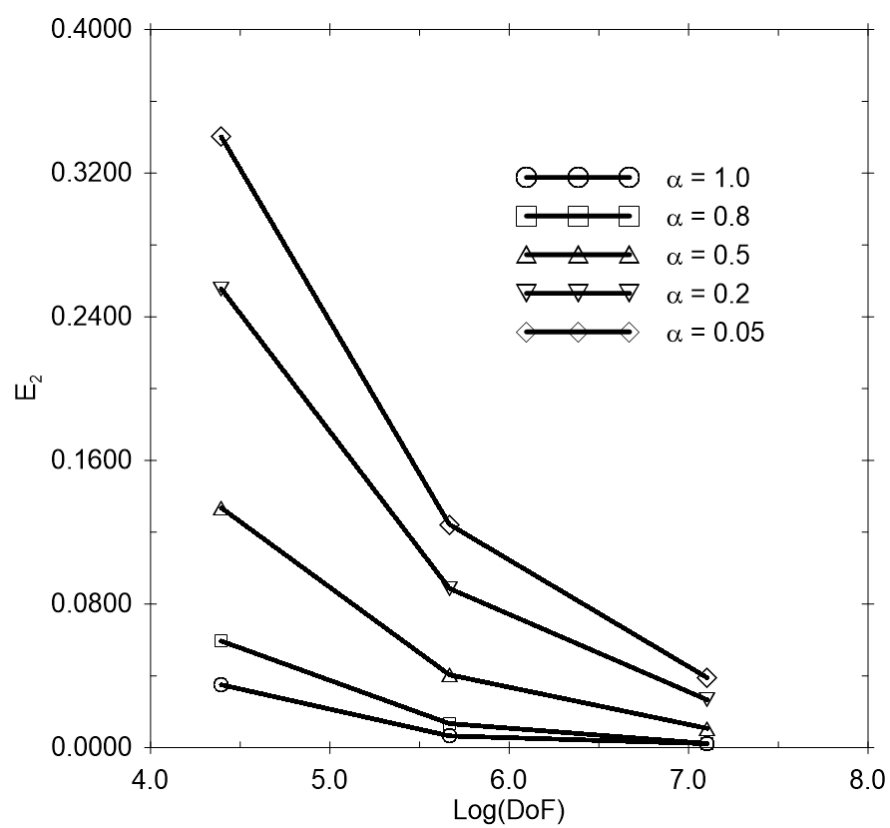


Figure 12

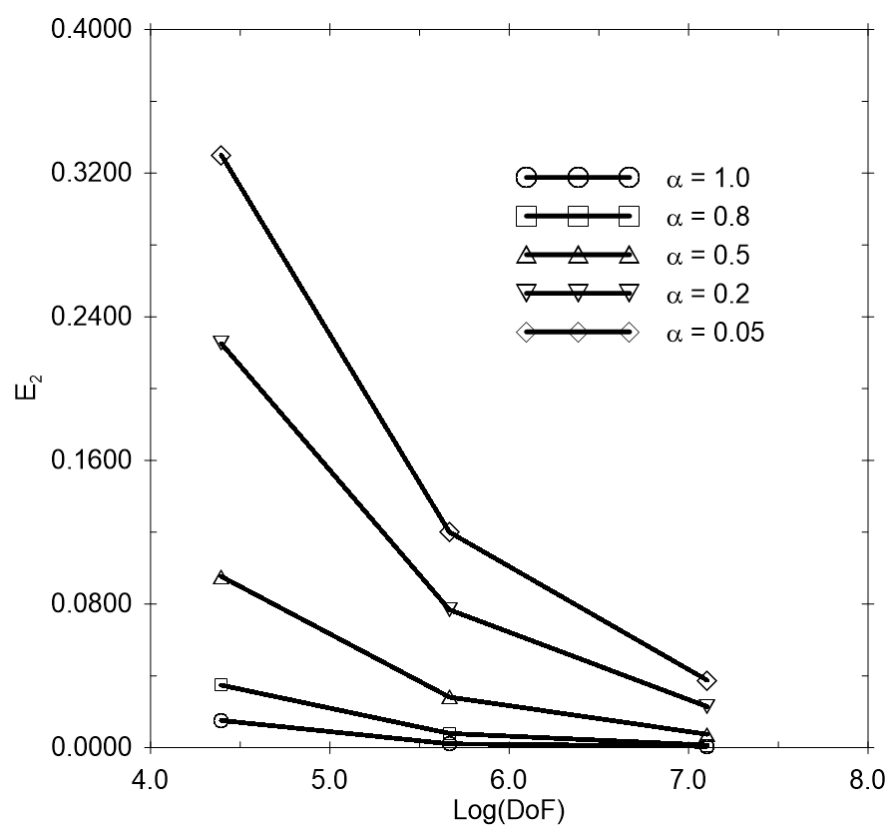


Figure 13

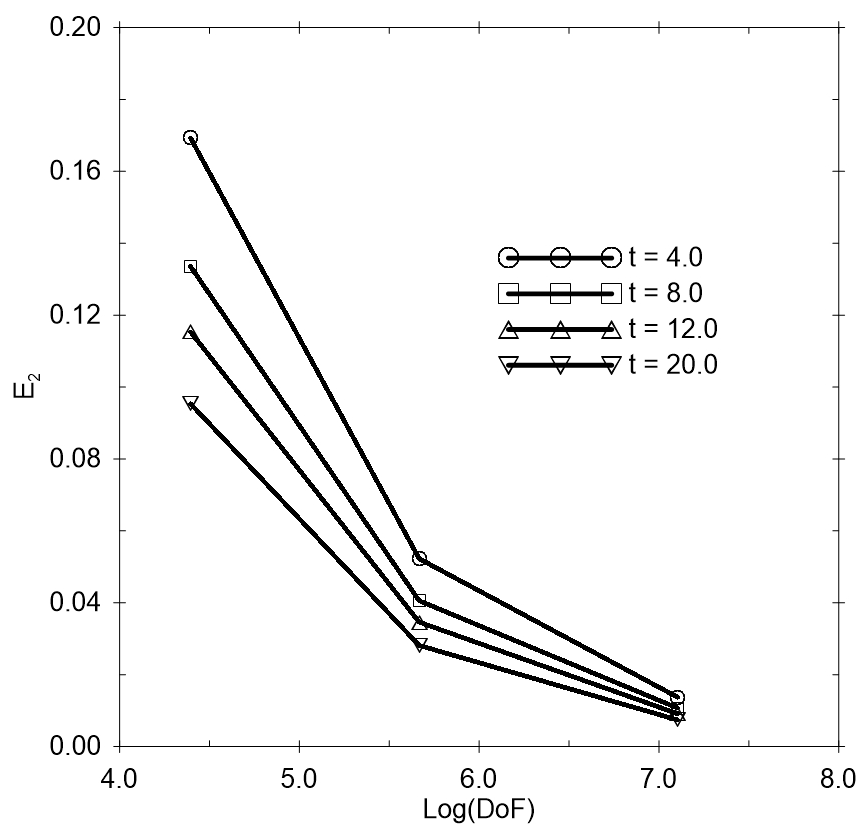


Figure 14

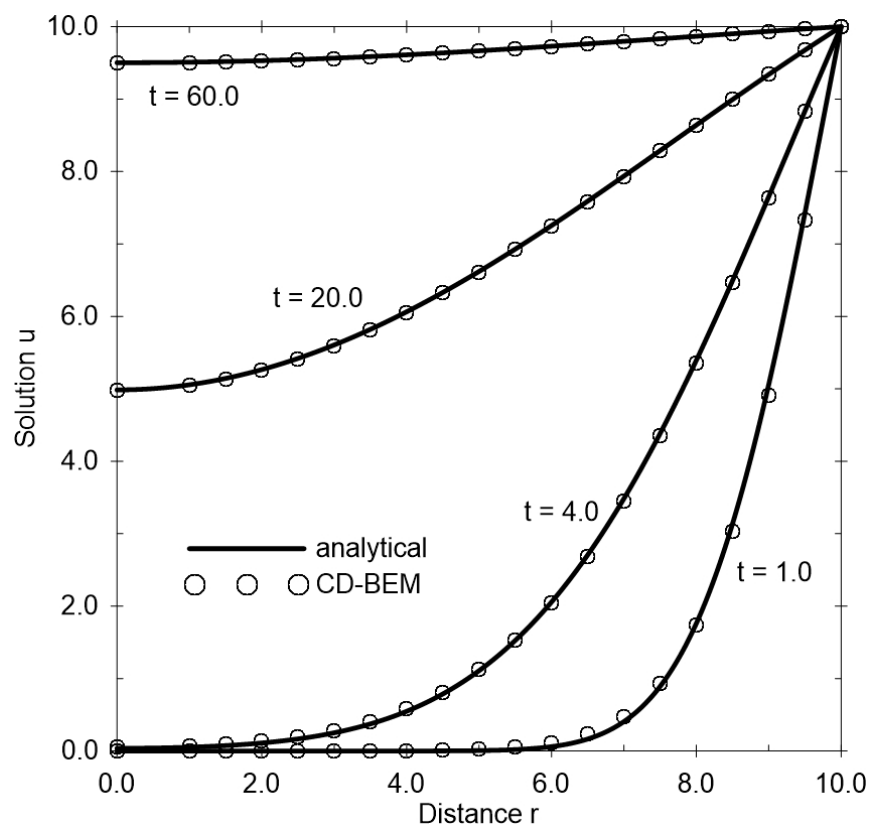


Figure 15

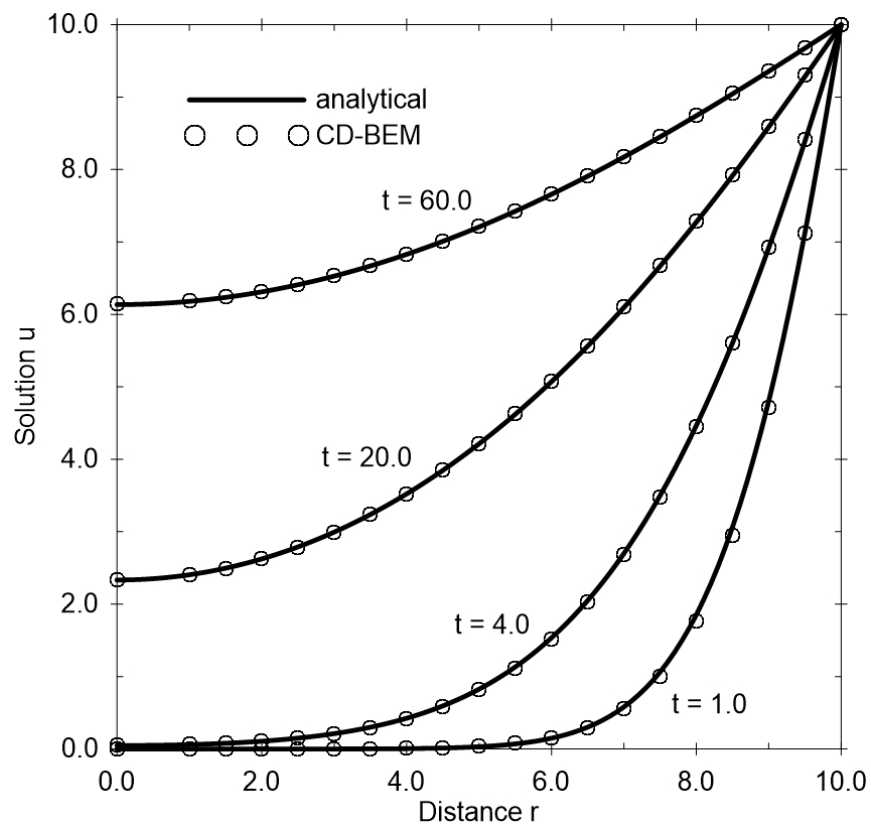


Figure 16

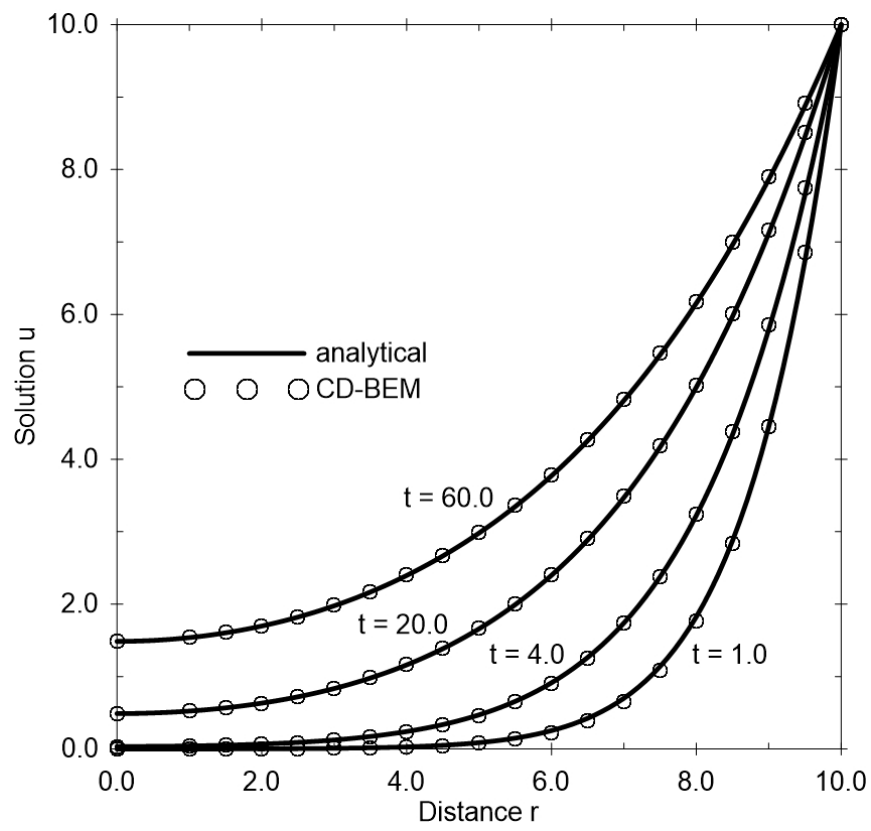


Figure 17

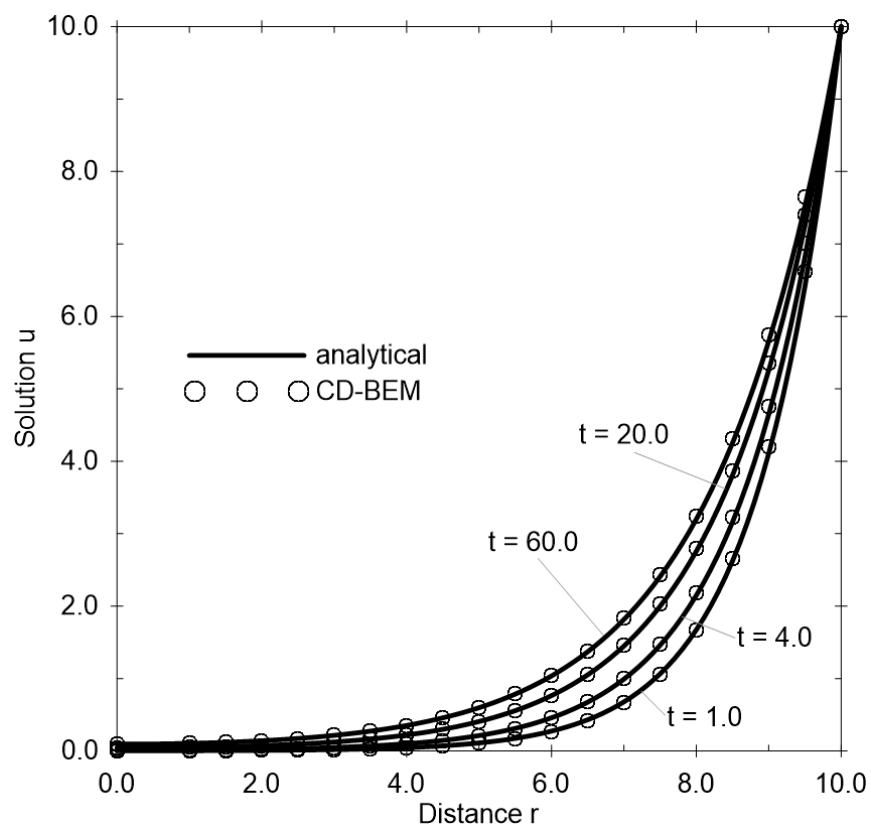


Figure 18

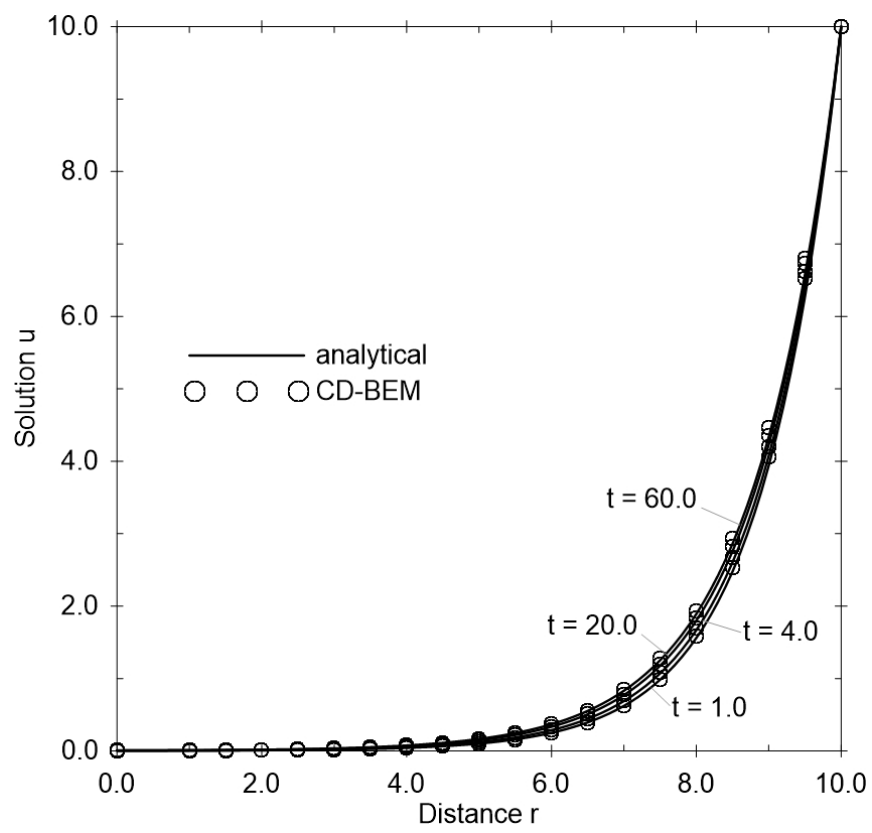


Figure 19

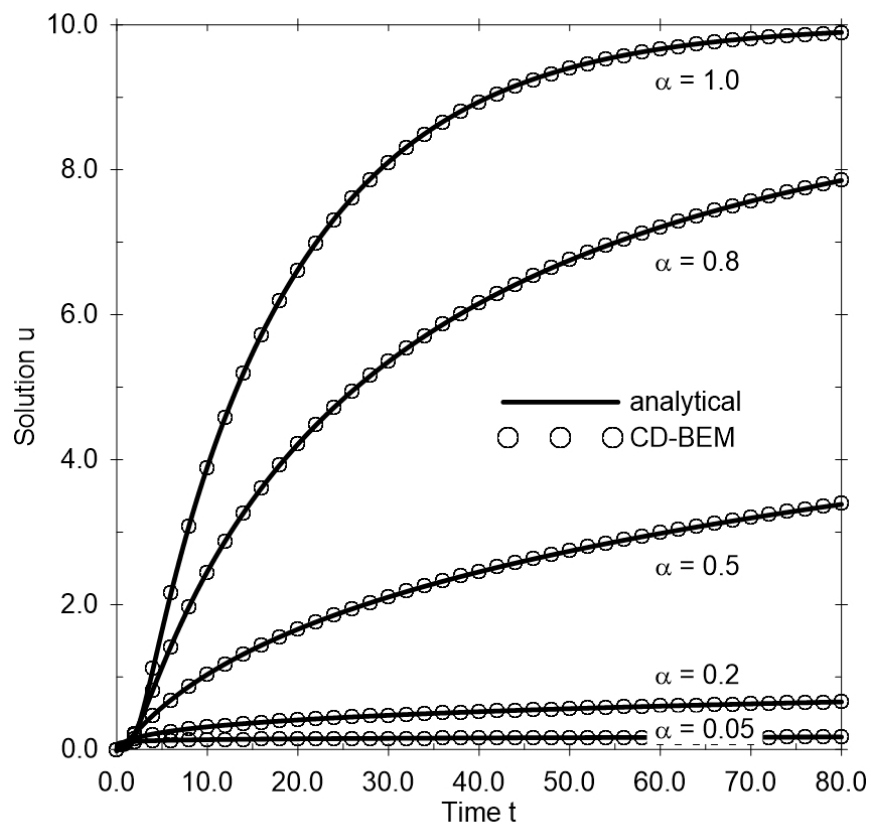


Figure 20

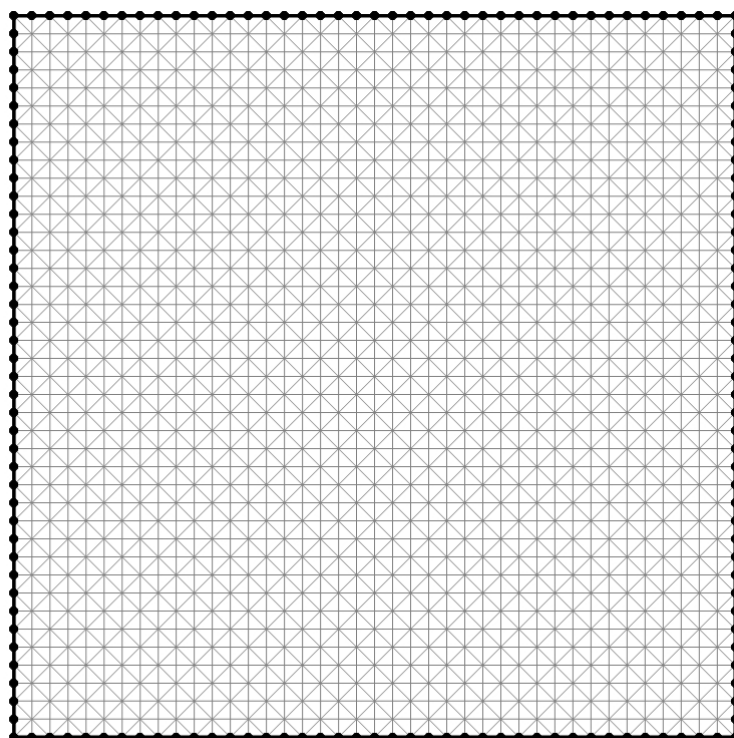


Figure 21

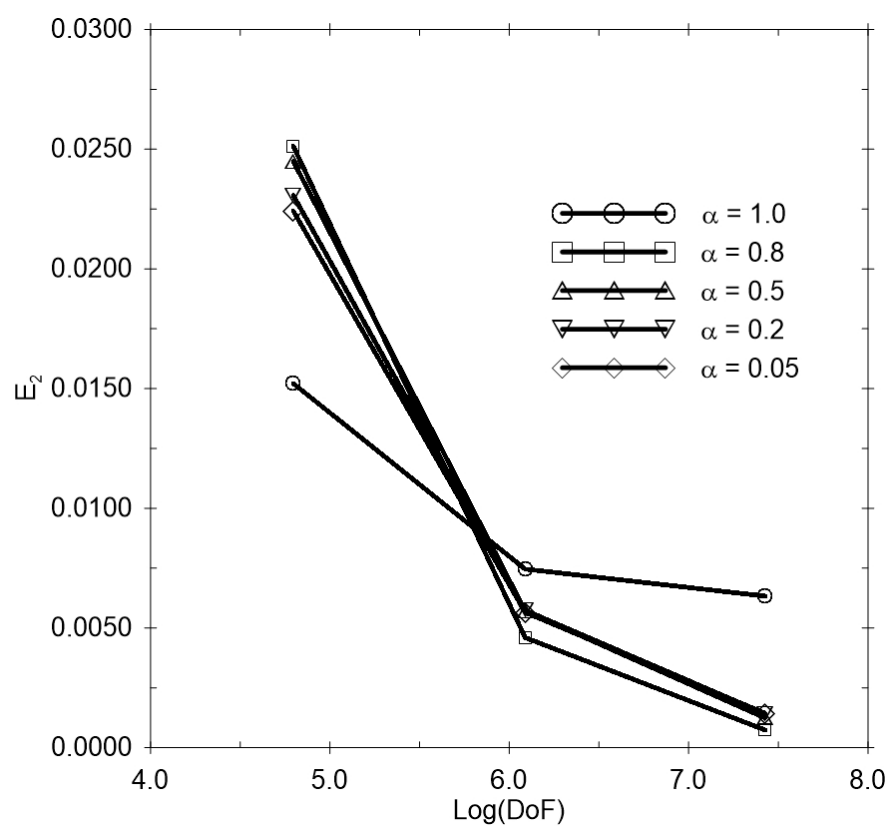


Figure 22

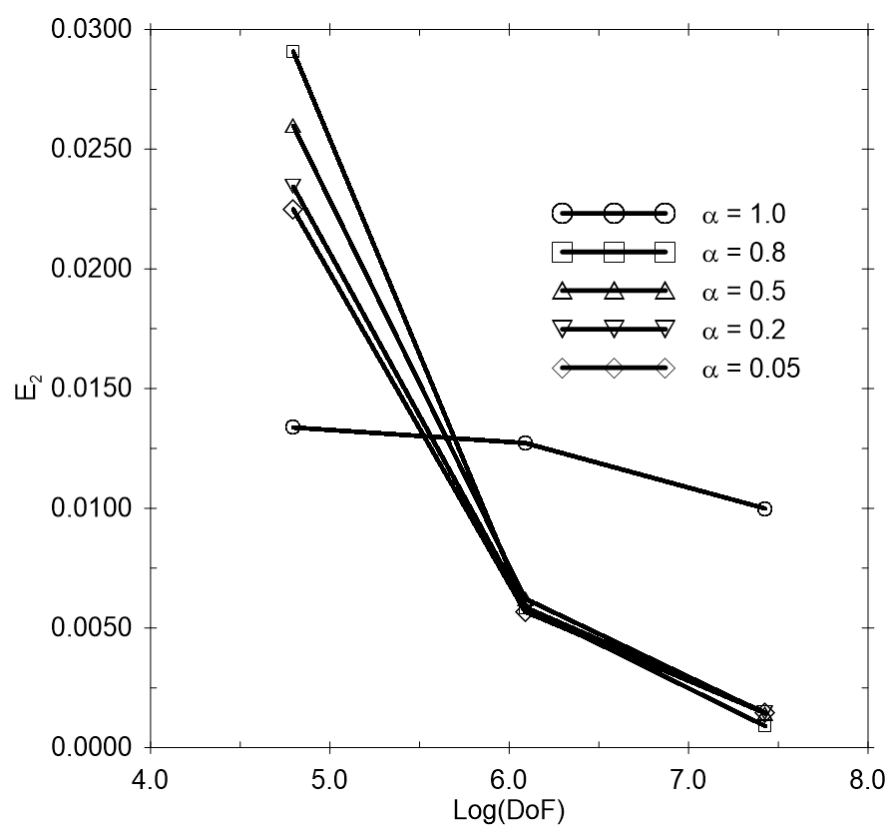


Figure 23

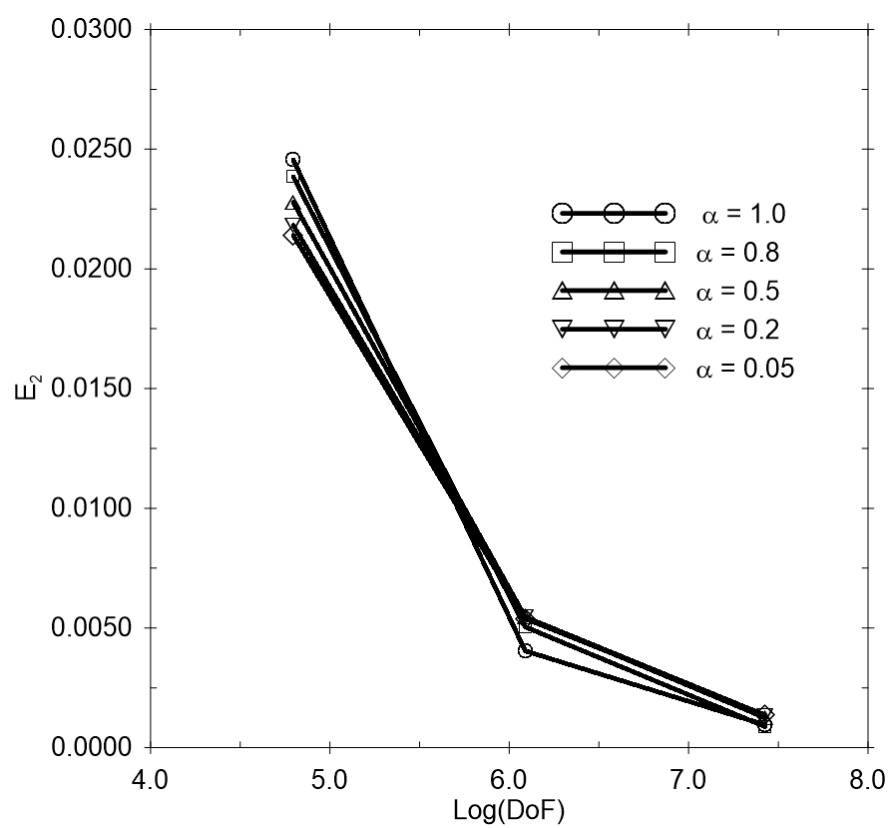


Figure 24

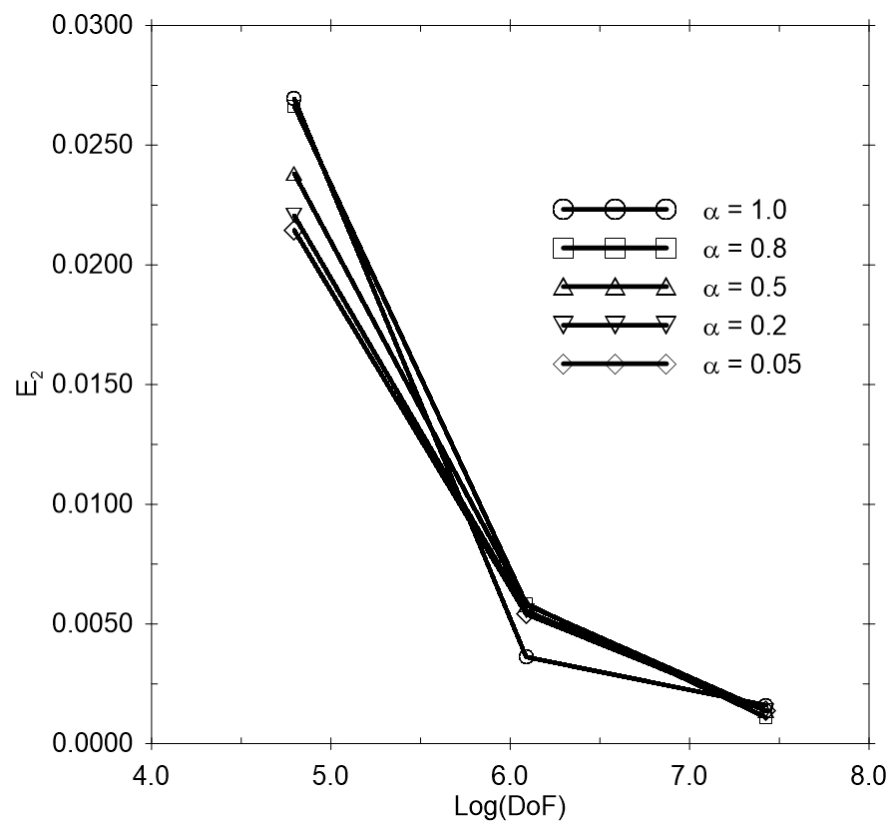


Figure 25

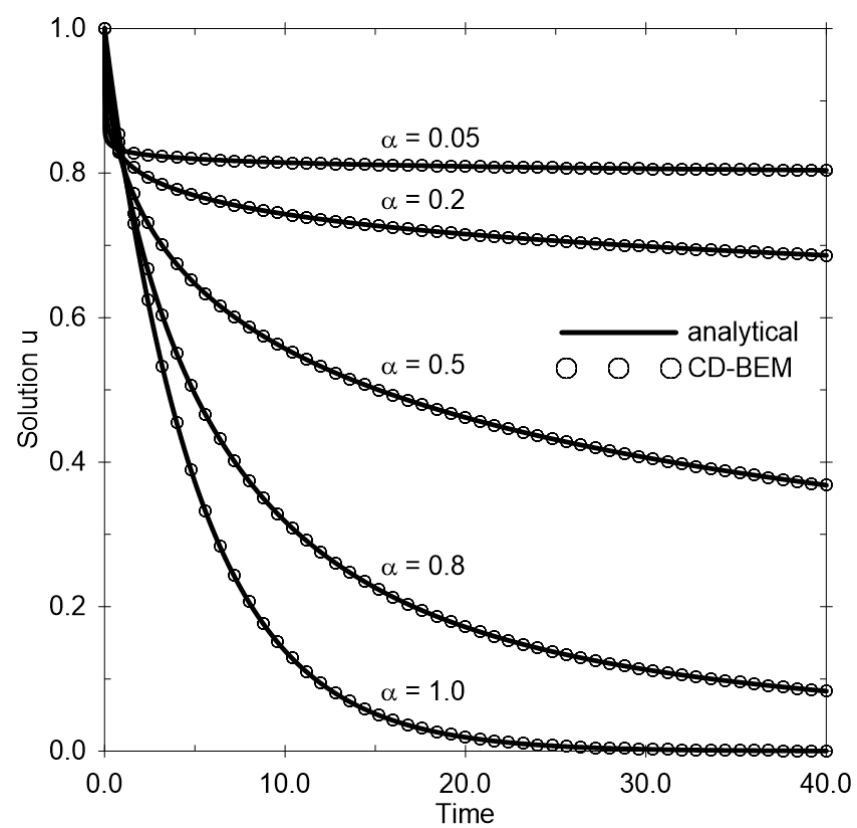


Figure 26

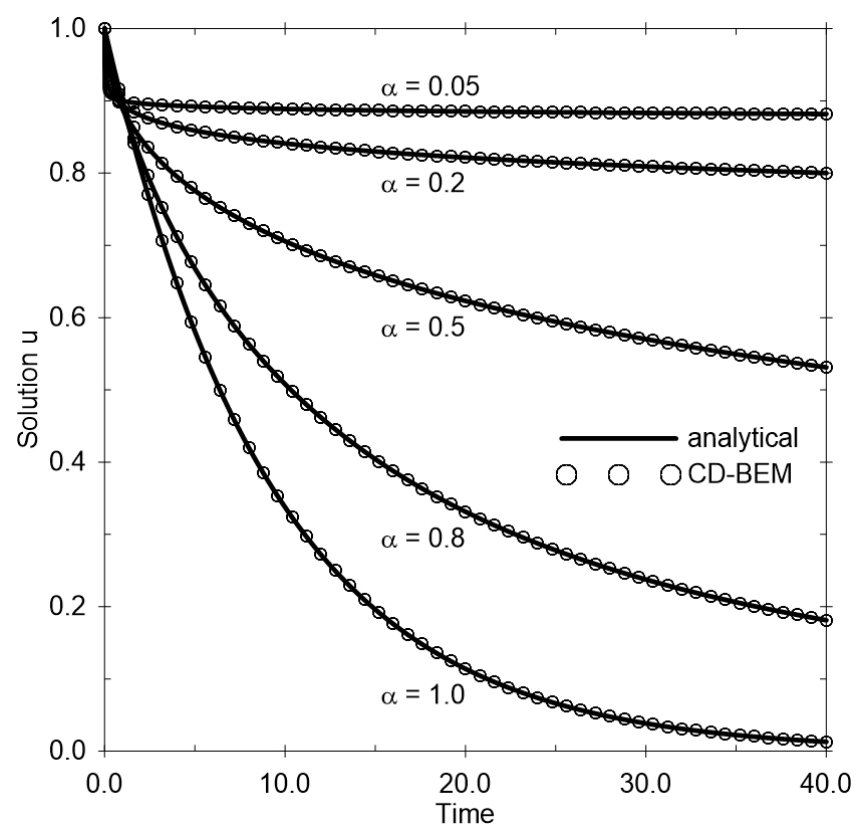


Figure 27

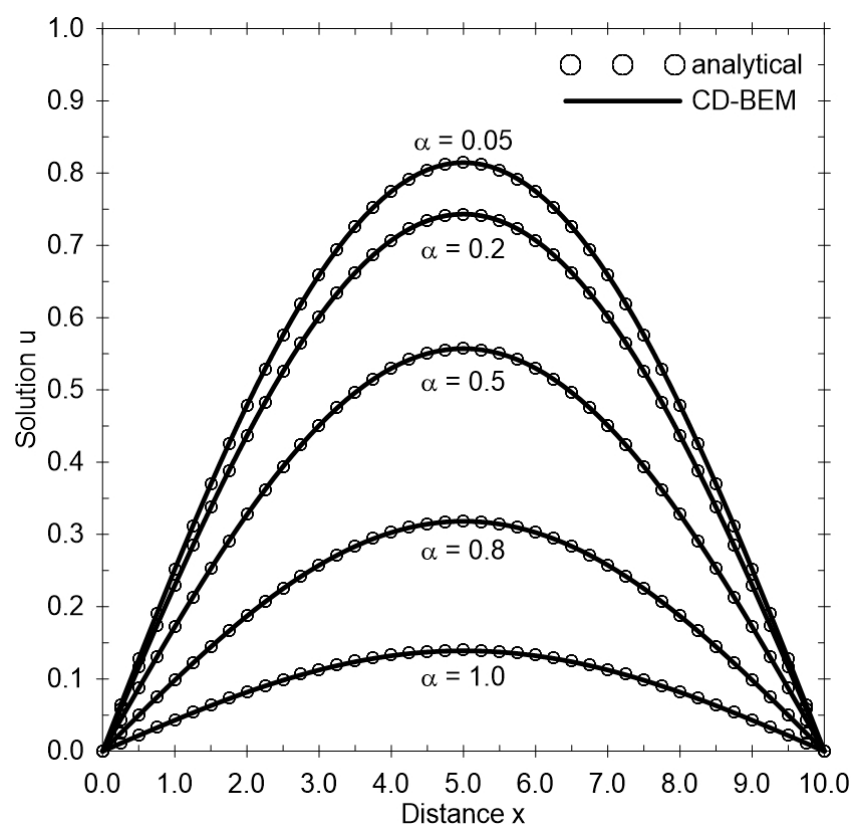


Figure 28

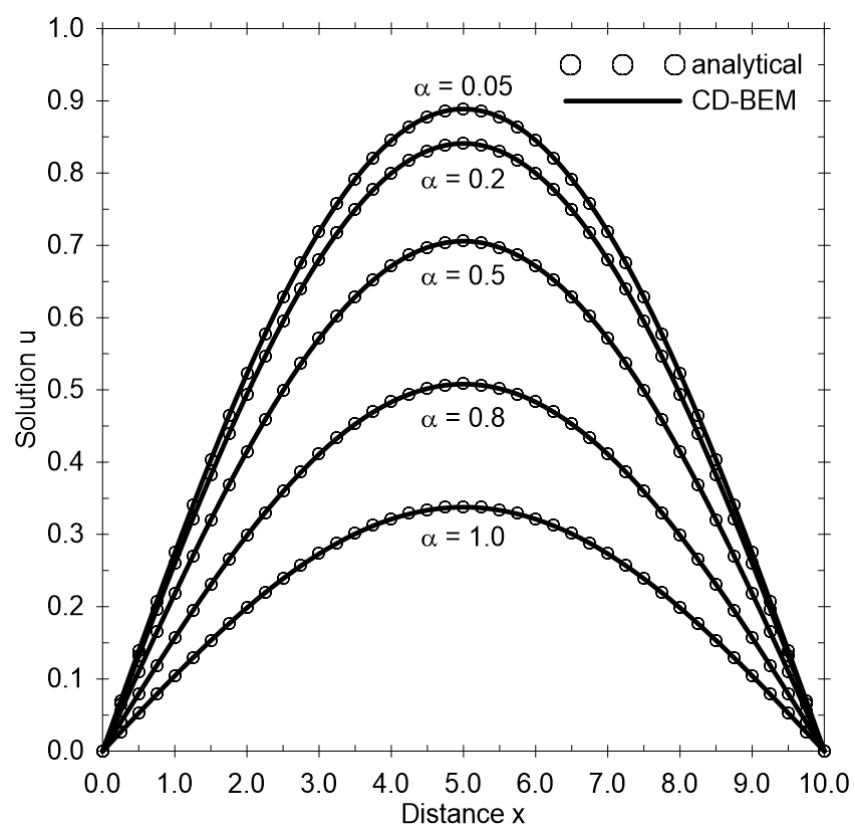


Figure 29

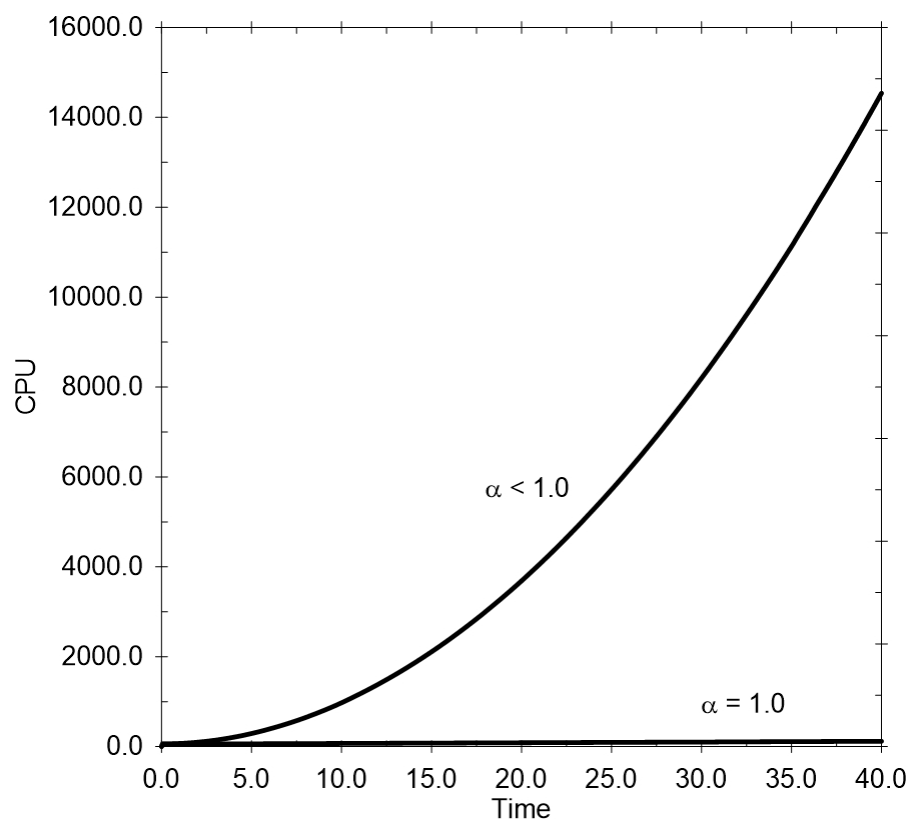


Figure 30